Condensed Matter Physics and Exactly Soluble Models

Selecta of Elliott H. Lieb

Edited by
B. Nachtergaele
J.P. Solovej and J. Yngvason

Springer

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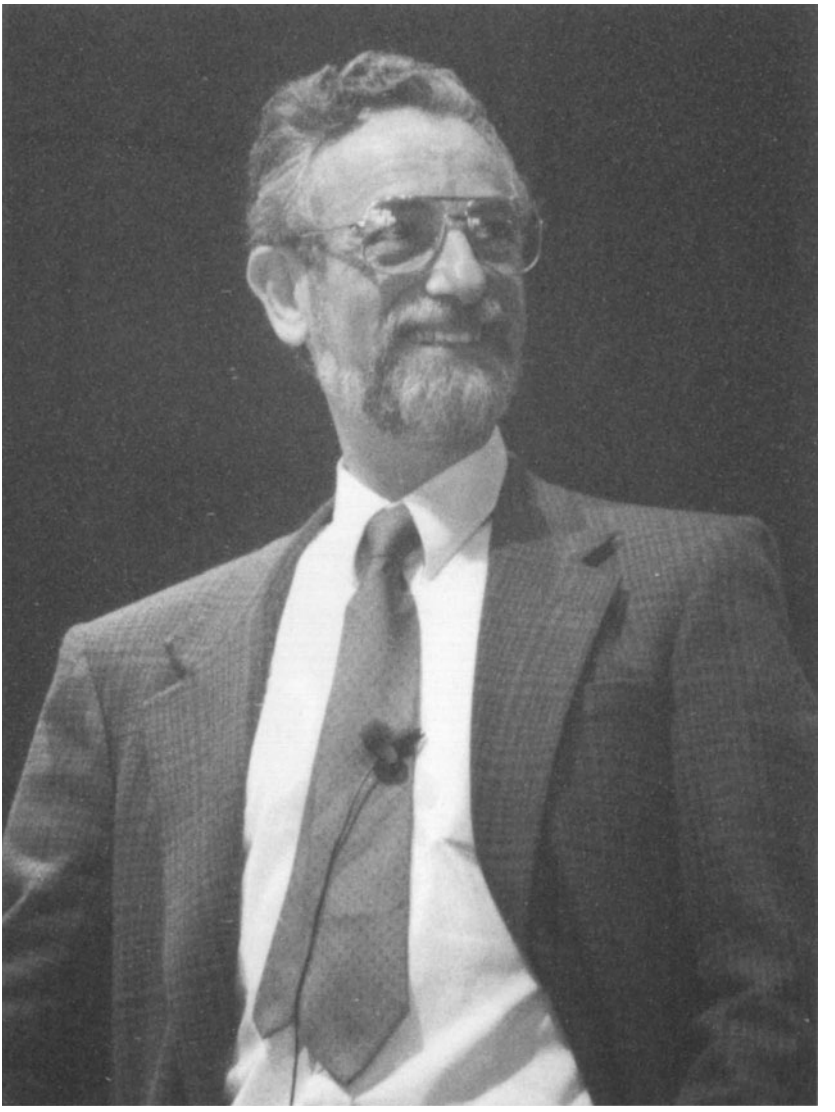

ELLIOTT H. LIEB

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Preface

This is the third Selecta of publications of Elliott Lieb, the first two being *Stability of Matter: From Atoms to Stars*, edited by Walter Thirring, and *Inequalities*, edited by Michael Loss and Mary Beth Ruskai. A companion fourth Selecta on *Statistical Mechanics* is also edited by us.

Elliott Lieb has been a pioneer of the discipline of mathematical physics as it is nowadays understood and continues to lead several of its most active directions today.

For the first part of this selecta we have made a selection of Lieb's works on *Condensed Matter Physics*. The impact of Lieb's work in mathematical condensed matter physics is unrivaled. It is fair to say that if one were to name a founding father of the field, Elliott Lieb would be the only candidate to claim this singular position. While in related fields, such as Statistical Mechanics and Atomic Physics, many key problems are readily formulated in unambiguous mathematical form, this is less so in Condensed Matter Physics, where some say that rigor is "probably impossible and certainly unnecessary". By carefully selecting the most important questions and formulating them as well-defined mathematical problems, and then solving a good number of them, Lieb has demonstrated the quoted opinion to be erroneous on both counts. What is true, however, is that many of these problems turn out to be very hard. It is not unusual that they take a decade (even several decades) to solve.

The second part of this volume is devoted to selecta of Lieb's work on *Exactly Soluble Models*. Exactly soluble models, often also called integrable models, is now widely considered as a research field in its own right. As such, it has fruitfully interacted with other branches of mathematics and physics (e.g., quantum field theory, Lie algebras and generalizations, combinatorics, dynamical systems, and algebraic geometry). Lieb's groundbreaking work in this area bridges the gap between an era where only a few awe inspiring exact solutions were known (notably Bethe's Ansatz for the Heisenberg chain and Onsager's solution of the Ising model), and the beginning of a flourishing field with many new developments following in quick succession. While this may seem like ancient history now, the pivotal role of Lieb's solutions of the ice problem, and the Fierz-Rys F-model and Slater's KDP model was clearly recognized at the time as revolutionizing the field.

A glance at the table of contents of this volume will impress anyone by the large number of ground breaking papers it contains. What motivated us to republish these papers in book form is much more than the historical interest they certainly have; they continue to be relevant today as one of the best sources to learn many subjects in mathematical physics. In conjunction with the other three

volumes of Lieb's *Selecta*, this collection of papers can indeed serve as an "awesome" course in mathematical physics.

We thank Wolf Beiglböck for his support and encouragement of this project and Sabine Lehr, Brigitte Reichel-Mayer and Sandra Thoms of Springer-Verlag for their invaluable help with the production.

Davis, Princeton, Vienna, April 2004

Bruno Nachtergaele
Jan Philip Solovej
Jakob Yngvason

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Commentaries

A Survey by the Editors

The following is a brief description of Elliott Lieb's papers on *Condensed Matter Physics* and on *Exactly Soluble Models*. The numbers refer to the publication list of Elliott Lieb, which appears at the end of this volume. Some of the papers that are not included in this volume *Condensed Matter Physics and Exactly Soluble Models* appear in the other Selectas of Elliott Lieb, namely *The Stability of Matter: From Atoms to Stars*, *Inequalities*, and *Statistical Mechanics*. The publication list shows which papers appear in which Selecta. The papers in this Selecta are additionally marked in boldface with their numbers as given in the table of contents. The numbers in square brackets refer to works by other authors, which are listed at the end of this survey.

A. Condensed Matter Physics

I. Correlated Electrons

19 (**XIV.1**), 39 (**XIII.2**), 48 (**I.1**), 194 (**I.2**), 209, 220 (**I.3**), 221, 222 (**I.4**), 226

Joaquin Luttinger [30] proposed a model of one-dimensional interacting fermions that was based on a model of Walter Thirring in quantum field theory [44]. Earlier, Sin-itiro Tomonaga [45] had similar qualitative ideas, but Luttinger was unaware of this. The virtue of the Thirring model formulation was that the model could be solved exactly; unfortunately, Luttinger made a mistake in his solution, one that had plagued early solutions of the Thirring model.

While preparing the Luttinger paper for reprinting in the Lieb-Mattis book *Mathematical Physics in One Dimension* Lieb and Daniel Mattis discovered the error and fixed it in 19 (**XIV.1**) with the invention of a boson field constructed from the fermionic density operators. This was the first time that "bosonization" appeared in the condensed matter literature. It has been used since in various calculations, both approximate and rigorous. This model is discussed again in the section on *Exactly Soluble Models*.

Another exactly soluble case, also discussed in the section on Exactly Soluble Models, is the one-dimensional Hubbard model, 39 (**XIII.2**), solved with Fa-Yueh Wu in the thermodynamic limit. After the solution was found, Ole Heilmann and Lieb thought of investigating the Hubbard model for 6 electrons on a ring of 6 sites, also known as the Pariser-Parr-Pople model of Benzene. It turned out that it was easier to solve for the eigenvalues as a function of the potential strength U on a computer than to try to use the complicated general solution. The results, in 48 (**I.1**), were surprising. After accounting for all the symmetries in the problem (i.e., symmetry operations, such as translation, that leave both the potential and kinetic energies invariant) many examples of eigenvalues that are degenerate (independent of U and of eigenvalues that cross were found). This contradicts the simple chemist's 'non-crossing rule'. (Eq. (70) has a sign error, which affects the labelling of some figures when they are inverted.)

The Hubbard model (in all dimensions) is treated in 194 (**I.2**), 209, 220 (**I.3**), 222(**I.4**). Paper 194 (**I.2**) proves that the ground state of the Hubbard model with

an attractive interaction ($U < 0$) has total spin $S = 0$ in its ground state for any filling with an even number N of electrons. For the $U > 0$ case and for a bipartite lattice with A sites on one sublattice and B on the other, this translates (by hole-particle symmetry) into $S = |A - B|$ for $A \geq 0$ and for $N = A + B$. The methodology used here is reflection positivity, but with reflections in spin space, not in ordinary space.

A variant of spin space reflection positivity in paper 226, with James Freericks, proves that (continuum) electrons interacting with phonons (e.g., the Holstein model) has $S = 0$ in the ground state.

Several groups had conjectured that the magnetic flux that minimizes the ground state energy of free electrons in two-dimensions in a half filled band is π through every plaquette. Paper 222 (**I.4**) uses reflection positivity (see the *Statistical Mechanics Selecta*) to prove this not only for free electrons but also for the Hubbard model with any U. Moreover, it is proved for any dimension (with flux π through every face of a hypercubic lattice). Lieb's proof was subsequently simplified by Bruno Nachtergaele and Nicolas Macris [31]. This result demonstrates a curious and poorly understood interaction between the effect of magnetic fields on orbital motion and the effect of the Pauli principle.

Paper 209, with Michael Loss and Robert McCann, shows that for a half-filled band the one-body density matrix has the property that it is constant on the diagonal (i.e., $\varrho(x, y)$ with $x = y$) even if the hopping matrix elements and the interaction strength U are spatially varying, even random. This non-intuitive result was known in the chemistry literature in the case $U \equiv 0$ (the Hückel model).

A review of rigorous results by Lieb and others on the Hubbard model is in 220 (**I.3**).

II. Peierls Instability

175 (**II.1**), 227 (**II.2**), 228, 229

The Peierls instability is the instability in the lattice spacing in a crystal caused by the fact that the electron hopping amplitude (in a Hubbard type model) between nearest neighbor atoms depends on the distance between the atoms. In the "spin-Peierls" problem the distance dependent interaction is that between spins in a Heisenberg type spin model. The idea, which goes back to Jones [17], is that the overall effect, when the electron number N equals the number of atoms, will be a breaking of translational symmetry from period one to period two (as observed in certain alloys), but not to a larger period or to chaos. Independently, Herbert Fröhlich [12] and Rudolf Peierls [37] made this a bit more rigorous in one-dimension, where they were able to calculate the new period (assuming that symmetry was broken only to period two) and under the three assumptions that the electron-electron interaction was zero, that the dependence of the hopping amplitude has a linear dependence and that the distortion energy a quadratic dependence on the atomic spacing.

The first rigorous findings for a one-dimensional model with the three Fröhlich-Peierls assumptions were in 175 (**II.1**), with Tom Kennedy, It was proved that symmetry is broken to period two, at most. It was also proved, however, that if

one omits the assumption of pure quadratic distortion energy then one can get further symmetry breaking, even for $N = 4$. This contradicts received wisdom.

The case of general dependence (of the hopping amplitude and distortion energy) on the atomic spacing and with the inclusion of an arbitrary non-zero electron-electron Hubbard type on-site interaction was taken up in 227 (**II.2**), with Bruno Nachtergaele. It is shown that for one-dimensional rings (including the spin-Peierls model) the symmetry breaking is always only to period two when $N = 4k + 2$ but more complicated breaking can occur when $N = 4k$. In the $N \to \infty$ limit, however, all cases reduce to period two.

The method used in the proof is reflection positivity. See the Selecta on *Statistical Mechanics* for a discussion and reprints on this topic. Papers 228, 229 contain reviews of these results.

III. Falicov-Kimball Model

172, 173, 174 (**III.1**), 268, 270 (**III.2**)

One approach to the Hubbard model is to study what happens if one of the two kinds of electrons, say the spin-down electrons, cannot hop (but, because of the Pauli principle, there cannot be two on one site). This was done in 174 (**III.1**), with Tom Kennedy, and only later was it realized that such a model had been proposed earlier by Falicov and Kimball for a different reason and with a non-rigorous treatment.

One can ask for the location of the $N_\downarrow$ fixed, spin-down particles that gives the lowest possible ground state energy for a given number $N_\uparrow$. The main conclusion reached in 174 (**III.1**) (172,173 are similar) is that for a for a cubic lattice of 2N sites for any U, and with $N_\downarrow = N_\uparrow = N$, the optimum choice is to place the fixed particles on one of the two checkerboard sublattices. Actually, the proof has an extension to any bipartite lattice. If the interaction U is negative we can think of the fixed particles as atomic nuclei and the result is that the system forms a periodic structure (whose period is $\sqrt{2}$ in the case of a cubic lattice). This is the only rigorous example of the formation of a periodic structure from quantum mechanics. The Pauli principle is crucial here.

It costs energy to move the fixed particles from the optimum configuration and 174 (**III.1**) examines the positive temperature Gibbs state one gets after integrating out the moveable particles. The result is very much like the Ising model: there is a phase transition from an ordered to a disordered state in two or more dimensions.

Paper 268 with James Freericks and Daniel Ueltschi, of which 270 (**III.2**) is a summary, shows a quite different aspect of the model. Assume, now, that the lattice is the cubic lattice and that $N_\downarrow + N_\uparrow < 2N$. Assume also that the interaction $U = +\infty$. Then, instead of the fixed particles forming a nice lattice they clump together in the ground state and leave a hole in which the up-spins move. The total energy is the bulk energy one would expect for a free, spinless electron gas plus a positive energy proportional to the surface area of the hole formed by the fixed particles. In short, there is phase separation. This fact had been predicted for some time and this paper proves it.

IV. Ordering of Energy Levels

9 (**IV.1**), 10 (**IV.2**), 201 (**IV.3**)

Sometimes it is possible to prove that the total spin S of the ground state of a system with spin (either a spin model or an itinerant electron model) is $S = 0$. It is even better if one can prove that $E(S)$, the lowest energy for total spin S, satisfies $E(S) \leq E(S+1)$. This was proved for the Schrödinger equation for one-dimensional particles in 9 (**IV.1**), with Daniel Mattis; the theorem was surprising [38] since Heisenberg's 'exchange theory' of ferromagnetism can predict the opposite ($S = N/2$) in this case. Paper 10 (**IV.2**) proves a similar result for antiferromagnetic Heisenberg spin models (all dimensions), which generalizes earlier results of Marshall. Many years later, the extension of the result in 9 (**IV.1**) to positive temperature was accomplished with Michael Aizenman in 201 (**IV.3**). The proof method was quite different from that of 9 (**IV.1**) however.

V. Laser Models

70, 71 (**V.1**), 72 (**V.2**), 73 (**V.3**), 83 (**V.4**)

The Dicke laser model, and variants of it, describes a simple system of two-level atoms interacting with a finite number of photon modes in a cavity. Paper 70, with Klaus Hepp, studies the equilibrium thermodynamics of this model and proves, among other things, that it can go spontaneously into a lasing state at low temperature. The methodology for proving this second order phase transition was very much improved in 72 (**V.2**) with the introduction of coherent states (which also permitted the treatment of more general models and the elimination of the 'rotating wave' approximation).

The next step is the time evolution of the laser model studied in 71 (**V.1**), which also introduces infinite reservoirs (pumping and damping) to which the laser model of N spins is connected. The dynamic stationary states can bifurcate from lasing to non-lasing as the parameters of the system are varied. Thus, the laser can take the chaotic energy it receives from the reservoir and turn it into structured motion. This is the first rigorous example of a quantum mechanical cuckoo clock. In the $N \to \infty$ limit the system is dissipative and self-oscillatory.

The macroscopic observables of order N satisfy nonlinear classical equations of motion, whereas the fluctuation observables, which are of order $N^{-1/2}$, satisfy linear equations with Gaussian random forces, as predicted by Onsager and others. Further results on suitable initial conditions, simplifications, etc about this dynamical system are in 73 (**V.3**), 83 (**V.4**).

VI. Quantum Spin Systems

8 (**XI.1**), 168 (**VI.1**), 176 (**VI.2**), 181 (**VI.3**), 182, 252 (**VI.4**), 253

Paper 8 (**XI.1**), which is discussed below under 'Exactly Soluble Models', contains a theorem, in appendix B, that a finite chain Heisenberg $S = 1/2$ antiferromagnet of length L has an excitation energy at most of order $1/L$ above the ground state. The question whether, in the thermodynamic limit, this implies no energy gap or whether it implies multiple ground states (in the C^* algebra sense

of local observables) is discussed in 168 (**VI.1**) with Ian Affleck. For the isotropic model there is no gap, as expected, but for the anisotropic model with dominant S^3 interaction there are two ground states.

In 176 (**VI.2**) (announcement) and 181 (**VI.3**), with Ian Affleck, Tom Kennedy and Hal Tasaki, the 'valence bond' model is introduced in which the interaction between two neighboring spin 1 atoms is $S \cdot T + \frac{1}{3}(S \cdot T)^2 + \frac{2}{3}$. This is twice the projector onto the state in which $S + T$ has spin 2. This model is now called the AKLT chain. It is possible to find a state in which $S + T$ has spin 0 or 1, but never 2 for a pair of neighboring spins and this is called a valence bond state. It is also shown that, unlike the spin 1/2 model (with $S \cdot T$ Heisenberg coupling), there is an energy gap to excited states, uniqueness of the ground state and exponential decay of truncated correlation functions in the thermodynamic limit. This is in line with Haldane's conjecture that the integer spin Heisenberg model has a gap whereas the half integer case has no gap (as proved in 168 (**VI.1**)). Motivated by the work of Affleck, Kennedy, Lieb, and Tasaki, Mark Fannes, Bruno Nachtergaele, and Reinhard Werner introduced the notion of Finitely Correlated State in [6]. In this work they prove the existence of a spectral gap above the ground state of a wide class of quantum spin chains of which the AKLT model is a special case.

Two- and higher dimensional models are also shown to have valence bond states when the spin S of each atom equals half the number of nearest neighbors and the Hamiltonian is the projector onto spin $2S$ for each pair. However, the existence of a gap has not been proved beyond one dimension, but paper 182, with Tom Kennedy and Hal Tasaki, does prove the exponential decay of truncated correlations and uniqueness of the ground state for $S = 3/2$ on the hexagonal lattice.

Papers 252 (**VI.4**), 253, with Peter Schupp, considers certain *frustrated* spin systems on two-dimensional lattices. These model the pyrochlore system in the real world. Using reflection positivity, it is proved that among the ground states there is one with total $S = 0$.

VII. The Polaron

3, 234 (**VII.1**)

The polaron model of Herbert Fröhlich [11] is a model of a conduction band electron interacting with the optical phonon modes of a crystal. The coupling is linear in this quantum mechanical model and it is one of the simplest, yet realistic examples of particles interacting with a quantized radiation field. It attracted much theoretical and practical interest. Earlier, Landau [27] and Pekar [39] had discussed a classical version in which the phonon modes are not quantized. For small coupling constant α (where the modified perturbation theory of Lee, Low and Pines [29] is available) the difference is profound, but for strong coupling there are so many phonons that they can be treated semiclassically and the semiclassical strong coupling result of Pekar ought to be exact. Pekar's result is in the form of a mean field integral equation for the ground state, whose energy equals $-C\alpha^4$. It was easy to see that Pekar's result gives an upper bound to the energy. The problem was to prove that it was also a lower bound (as $\alpha \to \infty$) and one of

the obstacles to doing this was the fact that any naive attempt yielded $-\infty$ instead of a finite number.

Feynman [7] produced an upper bound valid for all α using Wiener integrals and the Feynman-Kac formula, but it was larger than the Pekar bound [39] for large α. The first finite lower bound was in 3, with Kazuo Yamazaki. It had the right $\sim -\alpha^4$ behavior, but was about three times too big. Feynman's opinion at the time was that this was a waste of time and physicists should not bother with lower bounds. Fortunately, many people tried to find such a bound and, in the process, developed the theory. The large α ground state energy problem was finally solved by Donsker and Varadhan in 1983 using Wiener integrals and large deviation theory in infinitely many degrees of freedom [2]. This proof was hard to understand easily and a much simpler proof, 234 (**VII.1**), using more conventional concepts, and also including an error estimate, was found with Lawrence Thomas in 1997.

The problem of the effective (or renormalized) mass of this electron surrounded by a quantized field still awaits solution.

VIII. Interacting Bosons

5, 12 (**XII.1**), 13 (**XII.2**), 14 (**VIII.1**), 15, 16, 18, 91, 118, 188, 246, 254, 255, 257, 258, 265, 267, 273, 276, 278, 280, 282, 284, 285, 286, 288, 291 (**VIII.2**), 293 (**VIII.3**)

With the exception of 13 (**XII.2**) and 91, all these papers are about the ground state of Bose gases. Paper 5 shows how to compute the pseudo-potential for hard sphere bosons of Lee-Yang-Huang [28] to all orders, but it is not computationally useful. Papers 12 (**XII.1**) and 13 (**XII.2**) contain the solution to the one dimensional delta function Bose gas, which is discussed under Exactly Soluble Models. It is now much used to analyze some experiments on Bose gases in elongated traps (see 285, 286).

Papers 14 (**VIII.1**) outlines a program for computing the ground state energy of various gases in coordinate space instead of in momentum space, as all other schemes do. The energy is given in terms of the solution to an integro-differential equation. While it has not been made rigorous, this single formalism does agree with other theories in a variety of cases. Paper 15, with Arthur Sakakura, shows that it yields Foldy's result [8] for the charged Bose gas at *high* density (see also the discussion of 265 below); 16, with Werner Liniger, shows that it gives the exact result for the one-dimensional delta function gas at high density and is reasonably accurate at low density.

Paper 18 contains summer school lectures about what was known about the ground state problem in 1965. It is still relevant today.

Paper 118 discusses the two-component charged Bose gas and shows that thermodynamic stability does not hold; the energy would diverge as $-N^{5/3}$ if the positive particles have infinite mass. For finite mass, Dyson [4] showed in 1967 that the energy would diverge at least as badly as as $-N^{7/5}$ and this law was finally proved with Joseph Conlon and Horng-Tzer Yau in 188 in 1988. The exact coeffi-

cient $-CN^{7/5}$, conjectured by Dyson, took a longer time and was finally derived with Jan Philip Solovej in 288 in 2003.

A closely related problem is the one-component gas in a *fixed* neutralizing background. Here, the energy is of order $-N$, and the system has a nice thermodynamic limit as shown with Heide Narnhofer in 91. For high density ϱ the energy is $-CN\varrho^{1/4}$. Foldy [8] calculated C in a short paper in 1961 using Bogolubov's theory, but the $\varrho^{1/4}$ law was not proved until 1988 in 188. Finally, the coefficient C was established with Jan Philip Solovej in 2001 in 265.

The three-dimensional, low density Bose gas with a finite range repulsive two-body potential v is supposed to have a ground state energy $E(N) = 4\pi N\varrho a$, to leading order in ϱ, where a is the scattering length of v. Dyson [3] derived this as an upper bound in 1957, but it took until 1998 to derive this formula as a lower bound in 246 with Jakob Yngvason. The analogous, but strange looking result in two-dimensions, $E(N) = 4\pi N\varrho/\ln[\varrho a^2]$, proposed by Schick [40] in 1971, was proved in 258.

It was then possible to prove in 254, with Robert Seiringer and Jakob Yngvason, that the Gross-Pitaevskii equation is exact in the limit $N \to \infty$, $a \to 0$ with Na fixed. This equation is known to provide a good description of bosons in the traps used in experiments. The extension to two-dimensions was done in 263.

The existence of Bose-Einstein condensation in the ground state of a three-dimensional Bose gas has still not been proved. The only case in which it can be proved is the hard core lattice gas at half filling (see 94, 184). However, progress was made in 273, with Robert Seiringer, where it was proved that in the Gross-Pitaevskii limit there is not only condensation but it is 100%. This is the first general result of this kind. Further, superfluidity occurs in this limit (at least by one definition) as proved in 278 with Robert Seiringer and Jakob Yngvason.

It was conjectured, and recently proved experimentally, that if a trap is long compared to its width then the Bose gas should behave one-dimensionally and be described by the exactly soluble model in 12 (**XII.1**), 13 (**XII.2**). This was proved rigorously in 285, 286 with Robert Seiringer and Jakob Yngvason.

Paper 280, with Eli Eisenberg, proves that in a model of multi-component Bose gases (often called "bosons with spin") there is always a ground state that has maximum total spin. A bound on the 'susceptibility' at positive temperature is also derived.

Paper 291 (**VIII.2**), with Michael Aizenman, Robert Seiringer, Jan Philip Solovej and Jakob Yngvason rigorously analyzes a model that reproduces some of the recent, unusual experimental results about Bose gases in traps subjected to an "optical lattice". This "lattice" is a periodic, one-body potential produced by laser beams. The model problem is a gas of hard-core bosons on a lattice, and the imposed periodic potential has period two relative to this lattice. It is shown that the model has Bose-Einstein condensation for a weak periodic potential, but this is extinguished if the potential is stronger than some critical value. This conclusion, which agrees with experiment, fails for an "ideal" gas; the interparticle interaction is essential.

Papers 255, 257, 267, 276, 282, 286, 293 (**VIII.3**) contain reviews. Paper 293 (**VIII.3**) is an enlarged version of 267 and 276.

B. Exactly Soluble Models

The historical paper 237 *Some of the Early History of Exactly Soluble Models* is reprinted at the beginning of part B of this volume.

IX. The Six-Vertex Ice Type Models
29 (**IX.1**), 30 (**IX.2**), 31 (**IX.3**), 32 (**IX.4**), 33, 34, 40 (**IX.5**), 44, 52, 53, 56 (**IX.6**), 59, 62 (**IX.7**)

Ordinary ice is one of several substances that have a 'residual' (positive) entropy at $T = 0$, contrary to Nernst's "third law of thermodynamics". Pauling [36] modeled this by saying that each oxygen atom has a bond to four nearest neighbor oxygens and a hydrogen atom sits on each bond in one of two positions. This would give an entropy (per oxygen) $S = k \log 4$, which is too large. Pauling's "ice rule" is that locally there must be H_2O, i.e., exactly two of the four hydrogens connected to a given oxygen must be close to that oxygen. Then $S = kN^{-1} \log Z$ where N is the number of oxygens and Z is the number of hydrogen arrangements. Pauling made an approximate calculation of Z, which agreed admirably with the measured value and also with the numerical value of Z found by computer.

The two-dimensional version of the problem amounts to drawing an arrow on each edge of a square lattice with two arrows facing into each vertex and two facing out. John Nagle studied this problem in detail numerically [34]. Lieb solved it analytically in 29 (**IX.1**) (in the thermodynamic limit) by rewriting the problem as the calculation of the largest eigenvalue of a transfer matrix. The remarkably simple looking result (in the thermodynamic limit) is

$$\frac{S}{k} = \frac{3}{2} \log \frac{4}{3} .$$

Paper 32 (**IX.4**) contains the full details.

After this was done Andrew Lenard pointed out that the number of arrow configurations equals 3 times the number of ways of coloring the squares of the lattice with one of three colors so that adjacent squares have different colors. Thus, the ice solution also solves the three-color problem for the square lattice, asymptotically.

There are six possible arrow configurations at each vertex, so this is called a six-vertex model. The next step was to assign an energy to each of the six configurations, in which case Z now depends on temperature. The first model of this kind solved by the transfer matrix method was the Fierz-Rys F-model of an antiferroelectric in 30 (**IX.2**). It has an *infinite order* phase transition (i.e., the free energy is infinitely differentiable in T but there is one T value at which it is not analytic).

The next model was Slater's KDP model of a ferroelectric, in 31 (**IX.3**), which has a *first order* phase transition. Bill Sutherland provided the generalization to models intermediate between the extremes of the F and the KDP models [41]. It should be noted that all of these models can be solved exactly when an external field is added (i.e., an energy assignment that breaks arrow reversal symmetry)

and some very unusual physical phenomena emerge. This contrasts with the Ising and eight-vertex models, which can be solved exactly only in the symmetric, no field, situation.

Lieb's solution of the ice model and its generalizations was an impressive accomplishment and it had a direct impact on further developments in exactly solvable models in statistical mechanics. This is not the place to elaborate on the many interesting works in this field (see, e.g., [1]). Let us just mention one other outgrowth of the square ice solution, which is in combinatorics. In the early eighties William Mills, David Robbins, and Howard Rumsey [33] conjectured a formula for the number of alternating-sign matrices (i.e., matrices with entries 1, 0, or -1, and such that the non-zero entries have alternating signs in every row and column and so that the first and last non-zero value in every row and column is 1). This formula was proved by Doron Zeilberger [47]; the proof is long and involved. Shortly afterward, Greg Kuperberg [25, 26] realized that a much shorter and transparent proof could be given based on the fact that there is a simple correspondence between the set of ice configurations with so-called domain wall boundary conditions on an n by n lattice and the set of $n \times n$ alternating-sign matrices. A determinant formula for the partition function of the six-vertex model with such boundary conditions had been obtained by Anatoli Izergin [16] using results of Vladimir Korepin [24]. Kuperberg showed that the complicated determinant equaled the Mills-Robbins-Rumsey formula. The determinant formula is exact, even for a finite lattice. Izergin and Korepin were motivated by Lieb's solution of the ice problem and they looked for a variant that could be solved exactly for a finite system (and not just in the thermodynamic limit). Oddly, the domain wall boundary condition leads to a strictly lower entropy in the thermodynamic limit.

The connection between square ice configurations and combinatorial problems such as the alternating-sign matrix problem and coloring problems, as well as the determinant formulas for the six-vertex model, were known for several years by a number of people. For many years combinatorialists were working hard on a problem that was already solved! Perhaps Dyson would like to add this story to his list as another (small) example of a "missed opportunity" [5] due to lack of good communication between workers in different fields.

Paper 62 (**IX.7**), with Lawrence Glasser and Douglas Abraham, prove interesting analyticity properties, such as the existence of a natural boundary in the complex plane, for ice type models. Paper 52, with Douglas Abraham, T. Oguchi and Y. Yamamoto, and 53 with Abraham, solve a closely related problem which, physically, is sodium trihydrogen selenite.

Papers 33, 40 (**IX.5**), 44 are short synopses while 59, with Fa-Yueh Wu, is a very detailed survey of all known properties of the six-vertex models.

Paper 56 (**IX.6**), with Neville Temperley, created a mathematical industry. By expanding the transfer matrix setting of the ice type models (effectively doubling the number of sites in a unit cell), one can solve certain problems in two-dimensional percolation theory and certain 'coloring' problems. The diagonal transfer matrix is also introduced. Among the tools introduced to diagonalize the transfer matrix is an algebra of local operators, now called the Temperley-Lieb

algebra. The ideas in this paper and the Temperley-Lieb algebra itself have found numerous applications. To name just a few of the best known we mention subfactors of von Neumann algebras [18], knot invariants [19, 21], quantum groups, braid statistics in low-dimensional quantum field theory [9], and canonical bases of tensor products of irreducible representations of Lie algebras [21, 10].

X. Ising and Dimer Models

17 (**X.1**), 35 (**X.2**), 213

The solution of the two-dimensional Ising model of ferromagnetism by Onsager [35] in 1944 and Kaufman and Onsager [22, 23] in 1949 was a milestone in statistical mechanics because it proved that sharp phase transitions could actually occur in the framework of the Boltzmann-Gibbs formulation of equilibrium states. Unfortunately, this solution was viewed with awe by physicists, for it seemed very difficult. Today the solution is regarded as elementary and that is due mostly to 17 (**X.1**), with Theodore Schultz and Daniel Mattis, where it was shown that, in the right variables, the transfer matrix for the two-dimensional problem is essentially a one-dimensional problem of free fermions, which can be easily solved in terms of normal modes. The 'change of variables' that is needed is called the Jordan-Wigner transformation and it also appears in the XY model of antiferromagnetism (see 8 in Section XI on spin chains).

It later turned out that a similar analysis yields a solution of the two-dimensional dimer problem, 35 (**X.2**), originally solved by Kasteleyn [20] and Temperley-Fisher [43]. The monomer-dimer problem is, as one would imagine, closely related to the problem of the Ising model in a magnetic field, and both continue to defy solution. Paper 213 also contains information about dimer coverings on planar graphs.

XI. Spin Chains

8 (**XI.1**), 176 (**VI.2**), 181 (**VI.3**)

The study of one-dimensional quantum spin systems has a long history going back to Bethe and Hulthén. Paper 8 (**XI.1**), with Theodore Schultz and Daniel Mattis, was the first to analyze systematically the (anisotropic) XY model (in which only the 1 and 2 components of the spins interact). This model can be mapped onto a system of 'free' fermions. The other model analyzed in 8 (**XI.1**) is one in which the interactions switch between Heisenberg and Ising as one moves down the chain. This highly quoted paper also has useful formulas on diagonalizing quadratic forms in fermions and bosons.

Paper 181 (**VI.3**) gives the details of the AKLT model, and 176 (**VI.2**) is an announcement. It was discussed in the Condensed Matter Section VI on Quantum Spin Systems and is mentioned again here because it solves exactly the problem of the ground state of this spin system.

XII. Delta Function Bose Gas

12 (**XII.1**), 13 (**XII.2**)

These papers analyze the system of N bosons on a line of length L, interacting with a repulsive interaction $c\delta(x_i - x_j)$, with $c > 0$. The dimensionless constant in the problem is $\gamma = c/\varrho = cL/N$. (An attractive δ function interaction leads to a non-thermodynamic energy $\sim -N^2$.) The eigenfunctions of the Schrödinger equation have the "Bethe ansatz" form, i.e., they are simple superpositions of plane waves in each of the $N!$ regions in which the particle coordinates are ordered, but there is a discontinuity in the coefficients (but not in the wave function) when the ordering is changed. (This ansatz was rediscovered by Lieb while teaching at the university of Sierra Leone in 1961.)

Among the various findings, two stand out. One is that Bogolubov's approximate (but non-perturbative theory) is exact in the small γ limit (and it is reasonable even at large γ) – except for one thing. The excitation spectrum found in 13 (**XII.2**) has two branches, and not one as Bogolubov's theory predicts. One of the branches agrees with his theory for small γ; the other branch is absent in his theory. It is noteworthy, too, that the $\gamma \to 0$ limit is a singular and difficult limit for the exact solution but rather easy for the approximate Bogolubov approximation. The other major finding is that the Bogolubov theory starts by *assuming* nearly complete Bose-Einstein condensation, but the reality is that there is none in one-dimension. Nevertheless, the Bogolubov prediction for the energy and part of the excitation spectrum is correct at high density.

This exact solution now plays a role in the analysis of experiments on dilute gases in thin traps, as explained in the Condensed Matter Section VIII.

XIII. One-Dimensional Hubbard Model

36 (**XIII.1**), 39 (**XIII.2**), 279

The Bethe ansatz solution of the delta function Bose gas model did not imply a solution for the corresponding two-component fermion gas. The reason is that for bosons it is possible to reduce the problem to the region in x-space given by $0 \le x_1 \le x_2 \le \cdots \le x_N \le L$, but this is not possible for fermions. McGuire [32] solved the problem for $N - 1$ spin-up fermions and one spin-down fermion, but this particular choice can, indeed be reduced to just one subregion in which plane waves solve the equation. It was generally believed that the general problem could not be solved using plane waves until paper 36 (**XIII.1**), with Michael Flicker, in which the two spin-down particles problem was solved. This was done in a complicated way, but it showed that the general problem probably could be solved. It was Gaudin [13] and Yang [46] who independently saw the general solution.

The analogous problem on a lattice is the $U > 0$ Hubbard model. Using the Gaudin-Yang results, modified for the lattice case, Lieb and Fa-Yueh Wu reduced the ground state problem of the one-dimensional Hubbard model (in the thermodynamic limit) to a pair of coupled integral equations in 39 (**XIII.2**). These could be solved exactly for a half-filled band (i.e., $N = |\Lambda|$, where $|\Lambda|$ is the number of lattice sites. The most important physical result of this highly quoted paper is

that there is a jump in the chemical potential as one goes from $N = |\Lambda| - 1$ to $N = |\Lambda| + 1$, which means that the system is always an insulator at half filling as long as $U > 0$. There is no 'Mott' transition (other than at $U = 0$) from a conductor to an insulator as U is increased. In higher dimension a no-gap to gap transition is expected to occur at some finite $U \neq 0$. This unproved fact has been important in several areas, including high temperature superconductivity. The Lieb-Wu contribution is that a phase with a gap can actually occur. A similar phenomenon occurs in 291 (**VIII.2**) for bosons in an optical lattice. (See the commentary on **VIII.2**.)

Paper 279 revisits the integral equations and proves the result, promised in 39 (**XIII.2**), that they have a unique solution. The proof that the finite system (Bethe Ansatz) equations have a solution, and that these equations converge to the integral equations in the thermodynamic limit, has been recently completed by Pedro Goldbaum [14]. The continuity properties of the solution, needed to establish that they are, in fact, the ground state, have also been proved by him.

XIV. Luttinger Model

19 (**XIV.1**)

This is an exactly soluble model of interacting electrons in one-dimension. All the eigenvalues of the many-body problem can be computed. The model, which was discussed in the Condensed Matter Section I, was based on the Thirring model. The main feature, discovered in 19 (**XIV.1**), with Daniel Mattis, is "Bosonization", which is the appearance of bosonic modes in this fermionic problem. This was not seen in Luttinger's original paper [30].

Bruno Nachtergaele, Jan Philip Solovej, Jakob Yngvason

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A

Condensed Matter Physics

Part I

Correlated Electrons

VIOLATION OF THE NONCROSSING RULE: THE HUBBARD HAMILTONIAN FOR BENZENE*

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Abstract

The Hubbard Hamiltonian, while not one of the most successful models for π electrons in benzene, has been extensively investigated in the literature. As part of our general study of that model, we have computed all the energy levels for all values of the repulsion parameter—a task that has not been undertaken before. After extracting all the symmetry of the model we found, to our great surprise, many instances of permanent degeneracy of levels with different symmetry and also crossing of levels of the same symmetry. We can also demonstrate that there is no hidden symmetry to account for these effects. Since these results run counter to one of the oldest folk theorems in quantum chemistry, our otherwise uninspiring graphs may be of general interest.

I. The Model

The system to be considered consists of 2m electrons distributed among 2n identical, orthogonal orbitals that are regarded as localized at the vertices of a regular 2n-sided polygon. These electrons may be considered to be the π-electrons in certain cyclic compounds, primarily benzene,[1,2] or as the electrons in a ring of 2n hydrogen atoms using only the ls-orbitals,[3,4] or if n is large, as the conduction electrons in a one-dimensional metal.[5]

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The Hamiltonian to be used will be a rather simplified one with only two terms: a one-electron interaction between orbitals at neighboring sites and a two-electron interaction between electrons on the same site.[5,6] Such a Hamiltonian is known as the Hubbard Hamiltonian[5] and is one of the few points of contact between quantum chemistry and the many-body problem in solid-state physics. For large m and n, the ground state and low-lying excited states of the one-dimensional model have recently been solved exactly.[7] In an attempt to elucidate the nature of the higher states, especially their dependence on the two-electron repulsion parameter, we undertook a complete numerical study of the six-electron Benzene problem.

Numbering the orbitals around the polygon from 0 to 2n−1, and using $c^{\dagger}_{j\sigma}$ and $c_{j\sigma}$ for the creation and annihilation operators of an electron with spin σ in orbital number j, the Hamiltonian is

$$\mathbf{H} = \mathbf{T} + \mathbf{U} \tag{1}$$

$$\mathbf{T} = \mathbf{T}_{\uparrow} + \mathbf{T}_{\downarrow} \tag{2}$$

$$\mathbf{T}_{\sigma} = \mathbf{T} \sum_{j=0}^{2n-1} (c^{\dagger}_{j\sigma}\ c_{j+1,\sigma} + c^{\dagger}_{j\sigma}\ c_{j-1,\sigma}) \tag{3}$$

$$\mathbf{U} = \mathbf{U} \sum_{j=0}^{2n-1} c^{\dagger}_{j\uparrow}\, c_{j\uparrow}\, c^{\dagger}_{j\downarrow}\, c_{j\downarrow}\,. \tag{4}$$

Integers should be reduced modulo 2n into the interval [0, 2n−1].

There has been some debate in the literature whether the Hamiltonian (EQ. 1) adequately represents benzene. Linderberg and Öhrn's calculations[6,8] seemed to be affirmative, but not entirely so. Not only do some of the singlet states come out with symmetry assignments different from the generally accepted ones, but the purported agreement of the two triplet levels $^3E_{1U}$ and $^3B_{2U}$ with experiment is questionable inasmuch as the experimental data are quoted from Kearns,[9] who states clearly that they are only guesses partially supported by theory. Koutecky[10] was perhaps the first to challenge the appropriateness of H; the rejoinder[11,12] was that disagreements between theory and experiment were likely due to inadequate approximations and not to an inadequate Hamiltonian. Our detailed calculations of the energy levels (cf. section IV) suggest that both the Hamiltonian and the approximations are deficient. [Calculations using better Hamiltonians, in which all configurations in the configurational interaction are included, have indeed been carried out for benzene.[13]]

Although our original intention in undertaking these calculations was to investigate the Hubbard Hamiltonian in general and benzene in particular (2m = 2n = 6), our main conclusions now transcend our original interests. The surprising fact is that after the assignment of symmetry quantum numbers to all levels there are numerous cases of degeneracy of levels of different symmetry and, at the same time, cases of crossing of levels of like symmetry. A tentative explanation of these facts might be that there is additional symmetry that we have overlooked, but we can show this is not the case, at least if we understand symmetry operators in the generally accepted sense as being independent of the repulsion parameter, U. Since these results violate venerable dicta of quantum mechanics[14–21] we feel that a detailed presentation of our calculation may be of general interest.

II. The Symmetry

Normally, the first step towards diagonalizing a Hamiltonian is to find and use a sufficient amount of symmetry to reduce the matrices to be diagonalized to manageable proportions. It is not always necessary, and often not even desirable, to use all the symmetry. On the other hand, if one wants to disprove the noncrossing rule, it is necessary to know all the symmetry and to be able to make correct symmetry assignments to all the eigenvalues. To be certain that one has found all the symmetry seems difficult, but it is not impossible. In this section we shall content ourselves with finding most of the symmetry and defer the final resolution to section V.

All the symmetry operators will be written in terms of creation and annihilation operators and will turn out to have relatively simple representations in this notation; the necessary computation will therefore not be too complicated. The following definitions will be needed:

$$n_{j\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma} \tag{5}$$

$$n_{\sigma} = \sum_{j=0}^{2n-1} n_{j\sigma} \tag{6}$$

$$n = n_{\uparrow} + n_{\downarrow} \tag{7}$$

$$\begin{aligned} J_{j\sigma;k\tau} &= 1 - n_{j\sigma} - n_{k\tau} + c^{\dagger}_{j\sigma} c_{k\tau} + c^{\dagger}_{j\sigma} c_{k\tau} \\ &= \exp\left[\frac{i\pi}{2}\left(n_{j\sigma} + n_{k\tau}\right)\right] \exp\left[-\frac{i\pi}{2}\left(c^{\dagger}_{j\sigma} c_{k\tau} + c^{\dagger}_{k\tau} c_{j\sigma}\right)\right]. \end{aligned} \tag{8}$$

$n_{j\sigma}$ is the number operator that counts the number of electrons at site j with spin σ. $J_{j\sigma;k\tau}$ interchanges the orbitals $(j\sigma)$ and $(k\tau)$.

The symmetries are of three kinds: the symmetry of the polygon, the symmetry connected with the spin-coordinates, and symmetries associated with special features of the Hubbard Hamiltonian.

The spatial symmetry group, $C_{2n,v}$, can be generated by the operators C_{2n} and σ, which, respectively, rotate the polygon through $\frac{\pi}{n}$ and reflect it in a line through vertices 0 and n. They can be written as

$$\sigma = \prod_{\sigma=\uparrow,\downarrow} \prod_{k=1}^{n-1} J_{k\sigma;-k,\sigma} \tag{9}$$

$$\sigma' = \prod_{\sigma=\uparrow,\downarrow} \prod_{k=0}^{n-1} J_{k\sigma;2n-1-k,\sigma} \tag{10}$$

$$C_{2n} = \sigma\, \sigma'. \tag{11}$$

The symmetry of the spin coordinates can be found by using the operators S^2 and S_z:

$$S_z = \tfrac{1}{2}(n_{\uparrow} - n_{\downarrow}), \tag{12}$$

$$S_{+} = \sum_{j=0}^{2n-1} c^{\dagger}_{j\uparrow} c_{j\downarrow}, \quad S_{-} = S^{*}_{+}, \tag{13}$$

$$S_x = \tfrac{1}{2}(S_+ + S_-), \tag{14}$$

$$S^2 = \tfrac{1}{2}(S_-S_+ + S_+S_-) + S_z^2 . \tag{15}$$

We shall also need the operator

$$J^{(s)} = \prod_{k=0}^{2n-1} J_{k\uparrow\,;k\downarrow} \tag{16}$$

which interchanges spin directions. Using EQ. 8, $J^{(s)}$ can be written

$$J^{(s)} = \exp\left(i\,\frac{\pi}{2}n\right)\exp(-i\pi S_x). \tag{17}$$

From the definition of $J^{(s)}$ one easily gets

$$(J^{(s)})^2 = 1\,, \tag{18}$$

$$J^{(s)}S_z + S_z\,J^{(s)} = 0\,, \tag{19}$$

$$J^{(s)}\;S^2 - S^2\;J^{(s)} = 0\,. \tag{20}$$

These imply that if $\Psi_{S,M}$ is some eigenstate of S^2 and S_z with total spin S and z-component M, then

$$J^{(s)}\;\Psi_{S,M} = \Psi'_{S,-M}\,, \tag{21}$$

cf. APPENDIX (A.4). Expanding $\exp(-i\pi S_x)$ in powers of S_x and using EQ. 14, we see that $J^{(s)}$ does not mix different eigenstates of S^2 with the same eigenvalue of S_z, and hence

$$J^{(s)}\;\Psi_{S,0} = c_{S,m}\;\Psi_{S,0} \tag{22}$$

where $c_{S,m}$ is a constant that, for a fixed number, 2m, of electrons, depends only on S, and which, from (18), can be seen to be either 1 or -1. A trial $\Psi_{S,0}$ can be constructed as follows: An eigenstate of S^2 with $S = M$ and 2m electrons is

$$\left(\prod_{j=1}^{2S} c_{j\uparrow}^\dagger\right)\left(\prod_{j=2S+1}^{S+m} c_{j\uparrow}^\dagger\, c_{j\downarrow}^\dagger\right)|0> \tag{23}$$

The corresponding state with $M = 0$ is

$$\Psi_{S,0} = (S_-)^S\left(\prod_{j=1}^{2S} c_{j\uparrow}^\dagger\right)\left(\prod_{j=2S+1}^{S+m} c_{j\uparrow}^\dagger\, c_{j\downarrow}^\dagger\right)|0> \tag{24}$$

Acting on this state with $J^{(s)}$ gives:

$$\begin{aligned} J^{(s)}\Psi_{S,0} &= (S_+)^S\left(\prod_{j=1}^{2S} c_{j\downarrow}^\dagger\right)\left(\prod_{j=2S+1}^{S+m} c_{j\downarrow}^\dagger\, c_{j\uparrow}^\dagger\right)|0> \\ &= \left[\left(S_-\right)^S \prod_{j=1}^{2S} c_{j\uparrow}^\dagger\right]\left[\left(-1\right)^{m-S} \prod_{j=2S+1}^{S+m} c_{j\uparrow}^\dagger\, c_{j\downarrow}^\dagger\right]|0> \\ &= (-1)^m\;(-1)^S\;\Psi_{S,0}\,, \end{aligned} \tag{25}$$

which determines the value of $c_{S,m}$ in EQ. 22.

We turn next to the special symmetry of the Hubbard Hamiltonian. Most of this is pointed out in Lieb and Wu.[7] First, we define the operator $J_\sigma^{(o)}$, which changes the sign of the wave function for electrons of spin σ on odd sites. Likewise, $J_\sigma^{(e)}$ does the same thing for even sites.

$$J_\sigma^{(o)} = \prod_{k=0}^{n-1} (1 - 2n_{2k+1,\sigma})$$

$$J_\sigma^{(e)} = \prod_{k=0}^{n-1} (1 - 2n_{2k,\sigma}) \,. \tag{26}$$

The operator $J_\sigma^{(h)}$, which interchanges holes and particles for the spin direction σ, is:

$$J_\sigma^{(h)} = \prod_{k=0}^{2n-1} (c_{k\sigma}^\dagger + c_{k\sigma}) \,. \tag{27}$$

Using the commutation relations for the creation and annihilation operators, one can prove the following:

$$T_\sigma J_\sigma^{(o)} + J_\sigma^{(o)} T_\sigma = 0 \tag{28a}$$

$$T_{-\sigma} J_\sigma^{(o)} - J_\sigma^{(o)} T_{-\sigma} = 0 \tag{28b}$$

$$U J_\sigma^{(o)} - J_\sigma^{(o)} U = 0 \tag{29}$$

$$T_\sigma J_\sigma^{(h)} + J_\sigma^{(h)} T_\sigma = 0 \tag{30a}$$

$$T_{-\sigma} J_\sigma^{(h)} - J_\sigma^{(h)} T_{-\sigma} = 0 \tag{30b}$$

$$U J_\sigma^{(h)} + J_\sigma^{(h)} U = U n_{-\sigma} J_\sigma^{(h)} \tag{31}$$

$$n_\sigma J_\sigma^{(h)} + J_\sigma^{(h)} n_\sigma = 2n J_\sigma^{(h)} \,. \tag{32}$$

By taking suitable combinations of $J_\sigma^{(o)}$, $J_\sigma^{(e)}$, and $J_\sigma^{(h)}$, one gets the following operators:

$$J^{(o)} = J_\uparrow^{(o)} J_\downarrow^{(o)}, \; J^{(e)} = J_\uparrow^{(e)} J_\downarrow^{(e)} \tag{33}$$

$$J^{(h)} = J_\uparrow^{(h)} J_\downarrow^{(h)} \,, \tag{34}$$

$$I^{(o)} = J^{(o)} J^{(h)} = Z_\uparrow Z_\downarrow \,, \; I^{(e)} = J^{(e)} J^{(h)} \,, \tag{35}$$

$$Z_\uparrow = J_\downarrow^{(o)} J_\uparrow^{(h)} \,, \; Z_\downarrow = J_\uparrow^{(o)} J_\downarrow^{(h)} \,. \tag{36}$$

These operators satisfy:

$$I^{(o)} H - H I^{(o)} = U(2n - n) I^{(o)} \,, \tag{37}$$

$$Z_\uparrow H + H Z_\uparrow = U n_\downarrow Z_\uparrow \tag{38}$$

EQUATIONS 37 and 38 are among the types of generalized commutation relations treated in the APPENDIX. If $| 2m,M >$ be a state with 2m electrons and eigenvalue of S_z equal to M then one has:

$$I^{(o)} \, | \, 2m,M > = | \, 2(2n - m), \; -M > \,, \tag{39}$$

$$Z_\uparrow \, | \, 2m,M > = | \, 2(n - M), \; n - m > \,. \tag{40}$$

From the results of the APPENDIX (see also Koutecky[10,22,23] and Lieb and Wu,[7]) one concludes that if the states are eigenstates of H with energies E(2m,M), then

$$E(2m,M) = E(2(2n-m),\ -M) - U(2n-2m), \tag{41}$$

$$E(2m,M) = -E(2(n-M),\ n-m) + U(m-M). \tag{42}$$

EQUATIONS 40 and 42 tell us that the energy levels for $M = 0$, but arbitrary (even) electron number, 2m, can be obtained from those for $m = n$ only, provided these are known for all M. Correspondingly, the solutions for an odd electron number and $M = 1/2$ can be obtained from those with $m = n - 1/2$ and all M. From the theory of angular momentum, on the other hand, we know that for a fixed number of electrons the knowledge of all eigenvalues and eigenstates for one value of M is sufficient to find the eigenvalues and eigenstates for any numerically larger value of M. Consequently, solving the problem for $m = n$ and $M = 0$ immediately gives the solution for any even number of electrons, and solving the problem for $m = n - 1/2$ and $M = 1/2$, gives the solution for any odd number of electrons.

Finally, we shall investigate commutation relations between the symmetry operators we previously found and $I^{(o)}$ and $Z_\uparrow$ to see whether the use of the mapping (A.14) with $I^{(o)}$ for C or the mapping (A.20) with $Z_\uparrow$ for D implies any new symmetry. We find:

$$I^{(o)}\sigma = \sigma I^{(o)} \tag{43}$$

$$I^{(o)}\sigma' = \sigma' I^{(e)} = \sigma' I^{(o)}\ (-1)^n \tag{44}$$

$$I^{(o)}S_z = -S_z I^{(o)} \tag{45}$$

$$I^{(o)}S^2 = S^2 I^{(o)} \tag{46}$$

$$I^{(o)}J^{(s)} = J^{(s)}I^{(o)} \tag{47}$$

$$Z_\uparrow \sigma = (-1)^{n-1}\sigma Z_\uparrow \tag{48}$$

$$Z_\uparrow \sigma' = (-1)^n \sigma' Z_\uparrow\ (-1)^{n\downarrow} \tag{49}$$

$$Z_\uparrow S_z Z_\uparrow = (2n-n) \tag{50}$$

$$Z_\uparrow S_+ Z_\uparrow = \hat{S}_+ \equiv \sum_{2n-1}^{j=0} (-1)^j c_{j\uparrow} c_{j\downarrow} \tag{51}$$

$$Z_\uparrow S^2 Z_\uparrow = \hat{S}^2 = \tfrac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+) + (2n-n)^2 \tag{52}$$

$$\hat{S}_- = \hat{S}_+^* \tag{53}$$

$$Z_\uparrow J^{(s)} = J^{(s)}Z_\downarrow = (-1)^n J^{(s)} I^{(o)} Z_\uparrow \tag{54}$$

$$I^{(o)}Z_\uparrow = (-1)^n Z_\downarrow = Z_\uparrow I^{(o)} \tag{55}$$

Obviously, we have found an additional symmetry operator, $\hat{S}^2$.

III. The Diagonalization

In order to utilize the symmetry, we change to a new set of basic one-electron functions by introducing the momentum space creation and annihilation operators $d^{\dagger}_{p\sigma}$ and $d_{p\sigma}$ for $p = 0, 1, \ldots, 2n-1$:

$$d^{\dagger}_{p\sigma} = \frac{1}{\sqrt{2n}} \sum_{j=0}^{2n-1} e^{i\pi pj/n}\, c^{\dagger}_{j\sigma} \tag{56}$$

$$d_{p\sigma} = \frac{1}{\sqrt{2n}} \sum_{j=0}^{2n-1} e^{-i\pi pj/n}\, c_{j\sigma} \tag{57}$$

$$c^{\dagger}_{j\sigma} = \frac{1}{\sqrt{2n}} \sum_{p=0}^{2n-1} e^{-i\pi pj/n}\, d^{\dagger}_{p\sigma} \tag{58}$$

$$c_{j\sigma} = \frac{1}{\sqrt{2n}} \sum_{p=0}^{2n-1} e^{i\pi pj/n}\, d_{p\sigma} \tag{59}$$

Next, we introduce a vector notation for the basic 2m-electron wave function with μ spins up and ν spins down:

$$|\, r > = |\, p;q > = d^{\dagger}_{p_1\uparrow} \ldots d^{\dagger}_{p_\mu\uparrow}\, d^{\dagger}_{q_1\downarrow} \ldots d^{\dagger}_{q_\nu\downarrow}\, |\, 0 >, \tag{60}$$

together with the following standard convention of ordering the components:

$$\begin{aligned} p_1 &< p_2 < \ldots < p_\mu \\ q_1 &< q_2 < \ldots < q_\nu \end{aligned} \tag{61}$$

In vectors with components that are not in the interval [0, 2n−1], such components should be reduced modulo 2n into this interval. If the components of a vector are not in the standard order (EQ. 61), they should be permuted to obtain this ordering, and the wave function should be multiplied by −1 if the permutation is odd.

The wave functions (EQ. 60) are obviously already diagonal in n and S_Z, with eigenvalues $2m = \mu + \nu$ and $M = \frac{1}{2}(\mu - \nu)$. In general, no confusion should arise by just using the notation $|\, r >$ and assuming μ and ν to be given by the context.

The Hamiltonian can now be stated in matrix notation, which is necessary for computations:

$$H(r,r') = <r \,|\, H \,|\, r'> = 2T\, \delta(r,r') \sum_{k-1}^{2m} \cos\left(\frac{\pi}{n} r_k\right)$$

$$+ \frac{1}{2n} U\, \delta_{P,P'} \Delta(p,p') \Delta(q,q'). \tag{62}$$

We have used the following notation:

$$\delta(r,r) = \prod_{k=1}^{2m} \delta_{r_k, r_{k'}}, \tag{63}$$

$$P = \sum_{k=1}^{2m} r_k \text{ (modulo } 2n) , \tag{64}$$

$$\begin{aligned} \Delta(p, p') &= \mu \text{ if } p = p' \\ &= \epsilon(p,p') \text{ if the sets } \{p_j\} \text{ and } \{p'_j\} \text{ have } \mu - 1 \\ &\quad \text{members in common} \\ &= 0 \text{ otherwise.} \end{aligned} \tag{65}$$

In EQ. 65, $\epsilon = (-1)^d$, with d being the lexicographical distance between the component that occurs only in p and the component which occurs only in p'. EQUATION 62 follows easily from EQ. 1–4, 58, 59.

The transformation EQ. 56, EQ. 57 makes C_{2n} diagonal. Since the effect of C_{2n} is to change $c^\dagger_{j\sigma}$ to $c^\dagger_{j+1,\sigma}$, one easily gets

$$C_{2n}\, d^\dagger_{p,\sigma}\, C^{-1}_{2n} = e^{i\pi p/n}\, d^\dagger_{p,\sigma} \tag{66}$$

and, therefore,

$$C_{2n} \mid r > = e^{i\pi P/n} \mid r > . \tag{67}$$

Similarly, one finds:

$$\sigma \mid r > = \mid -r > , \tag{68}$$

where $-r$ means that the components of r are multiplied by -1;

$$J^{(s)} \mid p;q > = (-1)^{\mu\nu} \mid p;q > ; \tag{69}$$

$$I^{(o)} \mid r > = (-1)^{2m+P} \mid -\overline{(r + ne)} > , \tag{70}$$

where $+ne$ denotes adding n to each component of r, and $\bar{r}$ means that p and q are changed to the vectors consisting of the integers from 0 to $2n-1$, which are not represented in p, respectively q.

By using EQ. 68, 69, and 70, it is fairly easy to find linear combinations of the basic wave functions $\mid r >$, which are also diagonal under σ, $J^{(s)}$ and $I^{(o)}$, as long as this does not destroy the already obtained diagonalization with respect to S_z and C_{2n}. In any case, $I^{(o)}$ can, of course, be used only if $m = n$, since $I^{(o)}$ otherwise does not commute with H, according to EQ. 37.

The other restrictions imposed are that σ can be used only for $P = 0$ and $P = n$ and that $J^{(s)}$ and $I^{(o)}$ can be used only for $M = 0$ ($\mu = \nu$). $J^{(s)}I^{(o)}$ can, however, be used for all values of M. We shall use the symbols σ, $J^{(s)}$, and $I^{(o)}$ to designate the respective eigenvalues of σ, $J^{(s)}$, and $I^{(o)}$.

The treatment of S^2 will be different. With the eigenvalues of S^2 equal to $S(S+1)$, one has $S \geqq \mid M \mid$, so that for a given m and M it is possible to recognize which eigenvalues of H belong to a certain eigenvalue of S simply by diagonalizing H for all higher values of $\mid M \mid$. This is a particularly useful approach for an even number of electrons with $M = 0$, since in this case $J^{(s)}$ can be used to distinguish between even and odd values of S (as shown above), and, consequently, we can avoid diagonalizing the case $M = 1$.

$\hat{S}^2$ can, of course, be treated in the same manner as S^2. As we are interested in ($M = 0$, $m = n$) in this paper, however, it is much easier to make use of $Z_\uparrow$. If $U/2n$ be subtracted from the diagonal of H:

$$H' = H - \tfrac{1}{2}nU, \tag{71}$$

then the relation EQ. 38 is changed to an anticommutation relation for $m = n$ and $M = 0$, since in this special case $Z_\uparrow$ does not change m and M according EQ. 40:

$$H' Z_\uparrow + Z_\uparrow H' = 0 . \tag{72}$$

From EQ. 52 and A.4 we then have that if $\Psi_{\epsilon', s, \hat{s}}$ is an eigenstate of H′ with eigenvalue ϵ', an eigenstate of S^2 with eigenvalue $S(S+1)$, and an eigenstate of $\hat{S}^2$ with eigenvalue $\hat{S}(\hat{S}+1)$, then $Z_\uparrow \Psi_{\epsilon', s, \hat{s}}$ is also an eigenstate of these three operators, with the respective eigenvalues equal to $-\epsilon'$, $\hat{S}(\hat{S}+1)$, and $\hat{S}(\hat{S}+1)$. The assignment of the different values of the quantum number $\hat{S}$ to the different eigenvalues of H′ therefore follows immediately from the assignment of S to the eigenvalues of H′.

$Z_\uparrow$ can, however, be used further to facilitate the diagonalization of H′ in the case $m = n$, $M = 0$. When the symmetry (C_{2n}, σ, $J^{(s)}$, and $I^{(o)}$) has been used to make H′ block diagonal, application of the unitary transformation

$$H' \rightarrow Z_\uparrow H' Z_\uparrow \tag{73}$$

will transform each of these diagonal blocks of H′ either into minus one times itself or into minus one times some other block. In the latter case it is obviously sufficient to diagonalize one of the two blocks.

The change in the eigenvalues of C_{2n}, σ, $J^{(s)}$, and $I^{(o)}$ caused by the transformation (EQ. 73) can be found from EQ. 48, 49, 54, and 55. They are listed in TABLE I.

TABLE 1
CHANGES IN EIGENVALUES*

n Odd	n Even
$P \rightarrow P$	$P \rightarrow P + n$
$\sigma \rightarrow \sigma$	$\sigma \rightarrow -\sigma$
$J^{(s)} \rightarrow -J^{(s)} I^{(o)}$	$J^{(s)} \rightarrow J^{(s)} I^{(o)}$
$I^{(o)} \rightarrow I^{(o)}$	$I^{(o)} \rightarrow I^{(o)}$

*The changes in the eigenvalues of C_{2n}, σ, $J^{(s)}$, and $I^{(o)}$ under the transformation given in EQUATION (73) for $m = n$ and $M = 0$.

As a final simplification, we observe that EQ. 28 and 29 imply that the unitary operator $J^{(o)}$ transforms the sign of T and leaves U unaltered:

$$J^{(o)} H J^{(o)} = J^{(o)} (T + U) J^{(o)} = -T + U . \tag{74}$$

Consequently, it suffices to diagonalize H′ for $U \geqslant 0$ and $T \leqslant 0$. By choosing $U - T$ as the energy unit, the following conditions on the parameters U and T encompass the entire range:

$$T = -(1 - U) \tag{75}$$

$$0 \leqslant U \leqslant 1 . \tag{76}$$

The rest of the work can be left to the computer. The computations consist of four major parts, whose details may be found in REF. 24:

With O.J. Heilmann in Annals of the New York Academy of Sciences *172*, 584–617 (1971)

1. Using EQ. 68, 69, and 70 to find the desired set of basic wave functions, and then using EQ. 62 to find the matrices corresponding to T and to U in this representation.
2. Diagonalizing H′ for sufficiently many values of U in the interval (EQ. 76).
3. Assigning the correct values of S and $\hat{S}$ to the eigenvalues.
4. Presenting the results in an appropriate manner.

IV. The Numerical Results

The energy levels for $n = m = 3$—in other words, the π electron system of benzene—are plotted in FIGURES 1–15. The energies, in units of U—4T, are those of $H' = H - 3U/2$ in order to exhibit clearly the symmetry about zero given by EQ. 72 and A.4. In the case of $I^{(o)} = -1$, only the figures for even S are shown, since the figures for $S = 1$ can be generated by inverting the figures for S even according to TABLE I. The figures for $\hat{S} = 2$ are also not shown, as they can be found by inverting the figures for $S = 2$ according to discussion following EQ. 72. For $P = 3$ the figures for $S = 2$ and $S = 3$ are not shown, since the levels are simply five energies of $-U/2$ and one energy of $-3U/2$.

Finally, all the figures for $P = 0$ and $P = 3$ with $\sigma I^{(o)} = -(-1)^P$ have been omitted, since it turned out quite unexpectedly that all the energies with $(\sigma, I^{(o)}) = (-1, (-1)^P)$ were also represented with $(\sigma, I^{(o)}) = (1, (-1)^P)$ and the same values of S and P and that all energies with $(\sigma, I^{(o)}) = (1, -(-1)^P)$ were also represented with $(\sigma, I^{(o)}) = (-1, -(-1)^P)$. The degeneracy can not, of course, be proved numerically, but it was at least within a maximum deviation of 10^{-7}, which is to be compared with an estimated computational uncertainty of $6 \cdot 10^{-7}$. The supposedly degenerate eigenvalues are shown with dotted lines.

As may be seen from the figures, there are many violations of the noncrossing rule. This is, of course, the result of an arbitrary decision. When one has calculated energies as shown by the points of FIGURE 16, one can either choose to obey the noncrossing rule, as indicated by - - -, or to make the curves as smooth as possible, as indicated by ..... Since the above-mentioned unexpected degeneracy has already shaken our confidence in the supposed efficacy of symmetry, the authors have not hesitated to prefer the latter possibility as far as the noncrossing rule is concerned.

The corresponding symmetry representation under the spatial symmetry group C_{6v} is given in each case in order to facilitate comparison with other calculations and experiments. Further, FIGURE 17 shows the lowest energy level for $^1A_1$, $^1B_1$, $^1B_2$, $^1E_1$, $^1E_2$, and $^3B_1$. When it is compared with the normally assumed ordering of the experimentally found levels,[25]

$$^1A_1 < {}^3B_1 < {}^1B_2 < {}^1B_1 < {}^1E_1 \tag{77}$$

it is seen that the levels $^1E_1$ and $^1B_1$ are interchanged for $-U/T < 8$ and that if $-U/T$ exceeds 2, then the level $^1E_2$ moves from above $^1B_1$ to the interval between $^1B_2$ and $^1E_1$.

Finally, TABLE 2 contains a comparison among experimental values, our exact calculation with the Hamiltonian (EQ. 1), and the approximate calculations of Linderberg and Öhrn[6] using Hamiltonian 1. The choice

$$T = -2.869 \text{ eV}, \; U = 6.068 \text{ eV}, \tag{78}$$

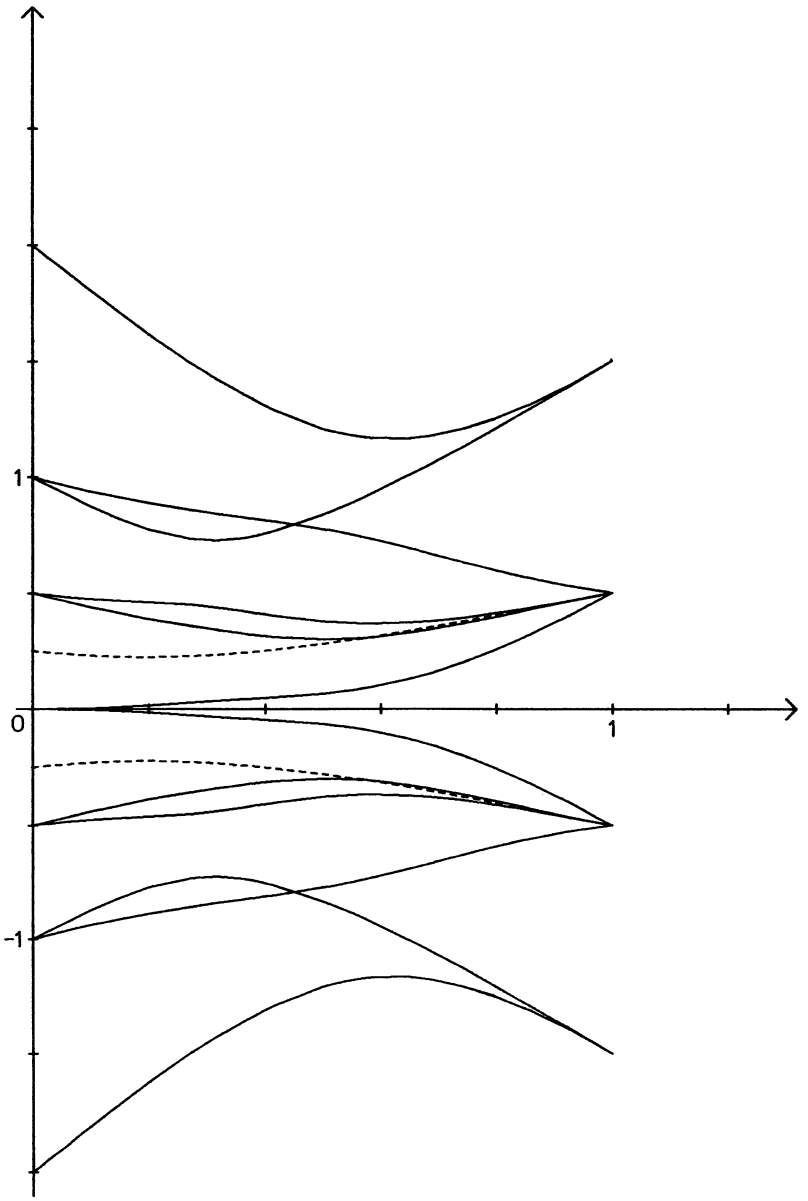

FIGURE 1. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (0, 0, 0, 1, 1)$, $^1A_1$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (0, 0, 0, -1, 1)$, $^1A_2$.

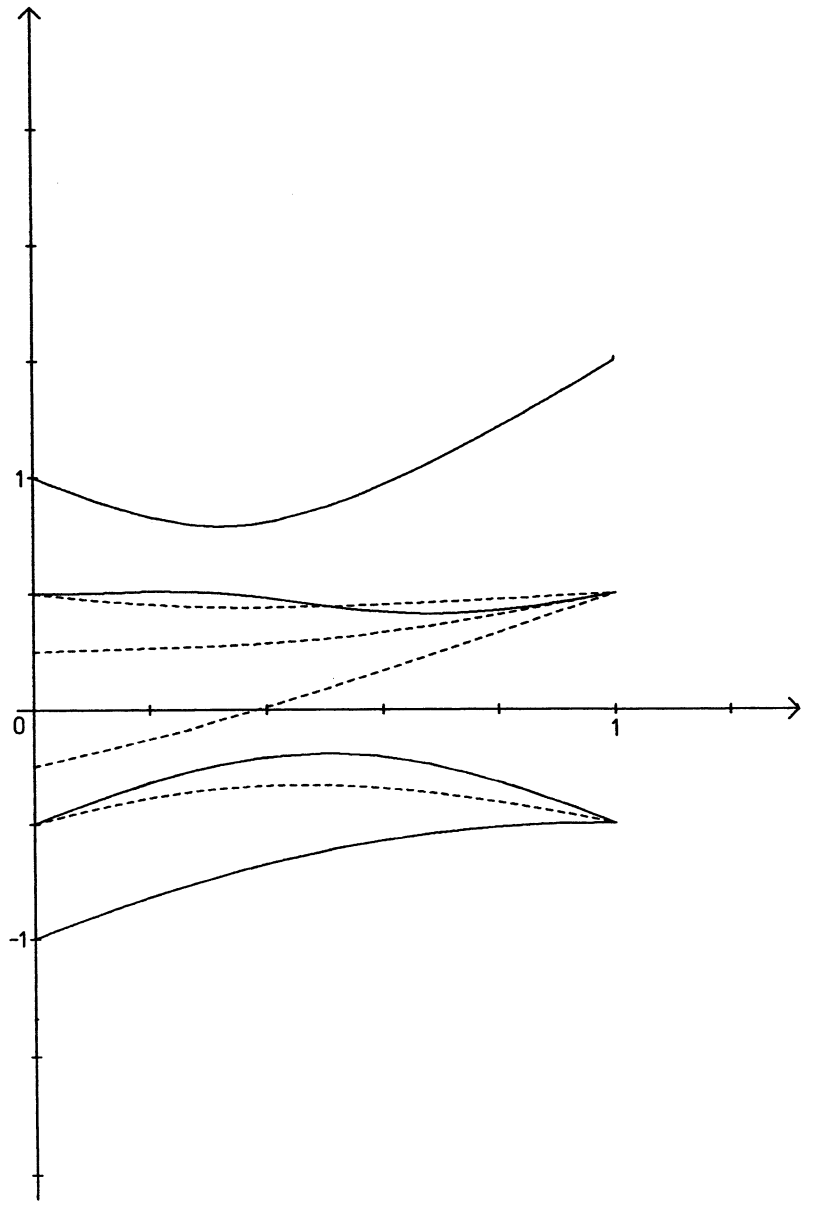

FIGURE 2. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(0)}) = (0, 0, 1, -1, -1)$, $^1A_2$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(0)}) = (0, 0, 1, 1, -1)$, $^1A_1$. Upside down the figure shows the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(0)}) = (0, 1, 0, -1, -1)$, $^3A_2$; - - - represents in this case the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(0)}) = (0, 1, 0, 1, -1)$, $^3A_1$.

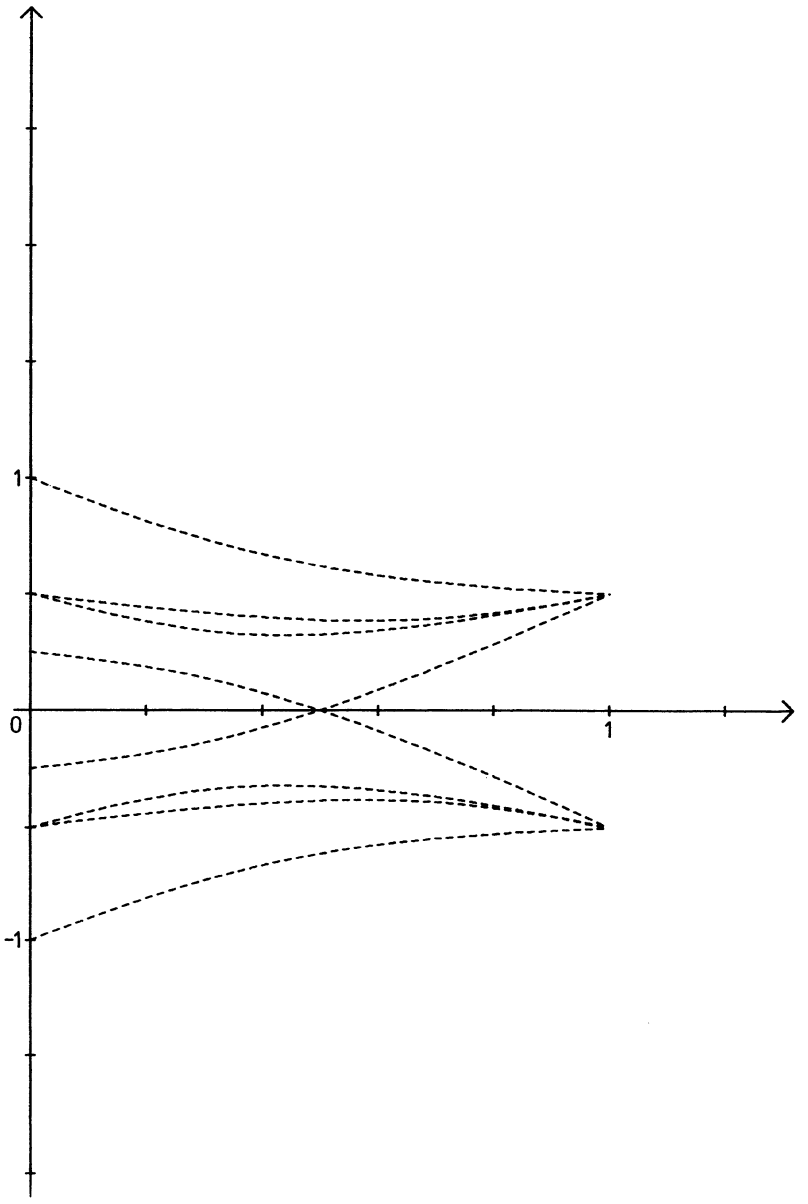

FIGURE 3. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (0, 1, 1, 1, 1)$, $^3A_1$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (0, 1, 1, -1, 1)$, $^3A_2$.

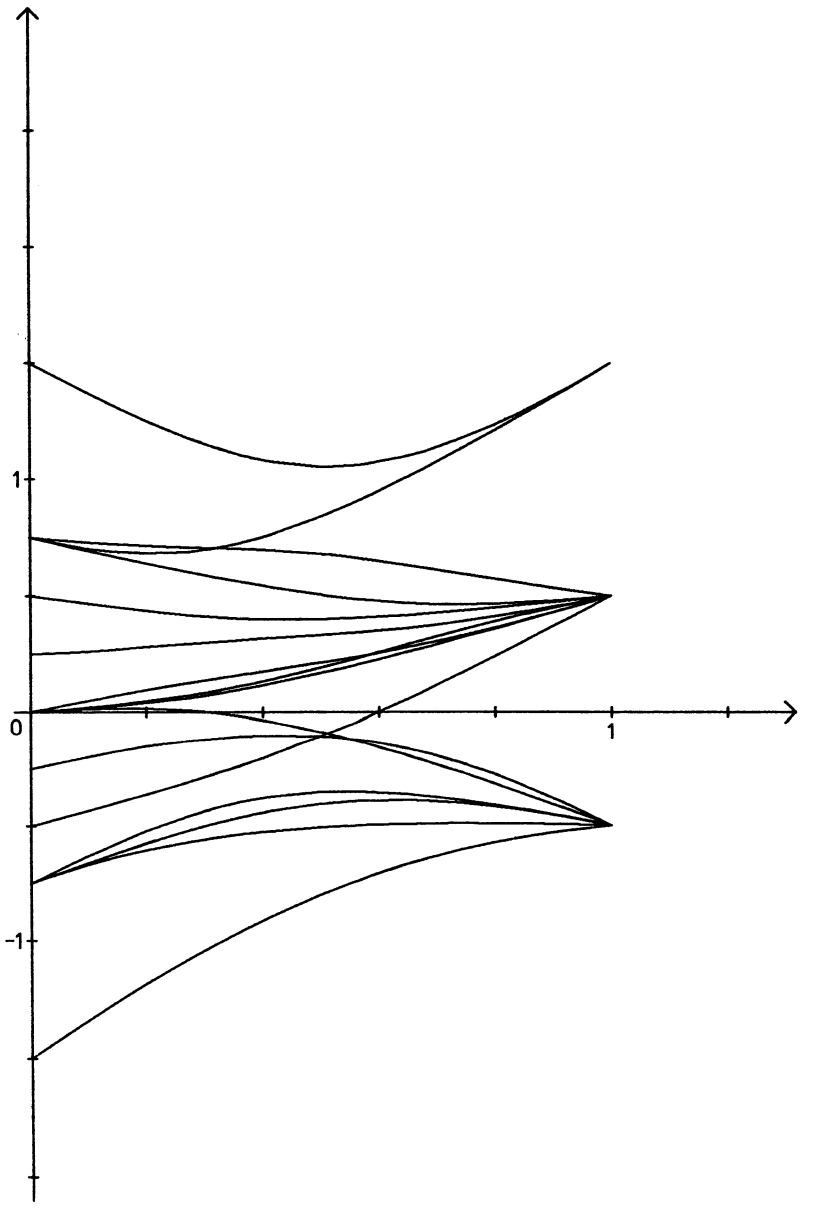

FIGURE 4. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (1, 0, 1, 1)$, $^1E_1$, in units of U-4T as a function of U. Upside down the figure shows the eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (1, 1, 0, 1)$, $^3E_1$.

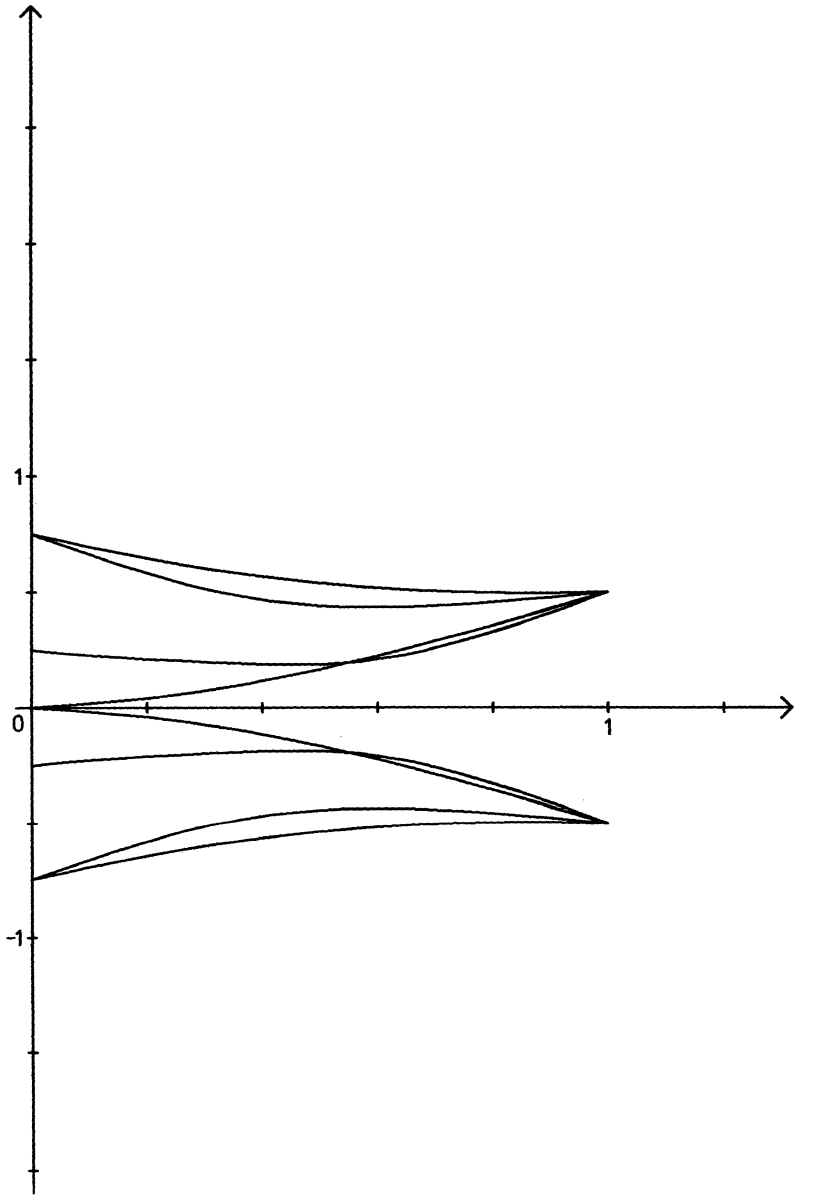

FIGURE 5. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (1, 0, 0, -1)$, $^1E_1$, in units of U-4T as a function of U.

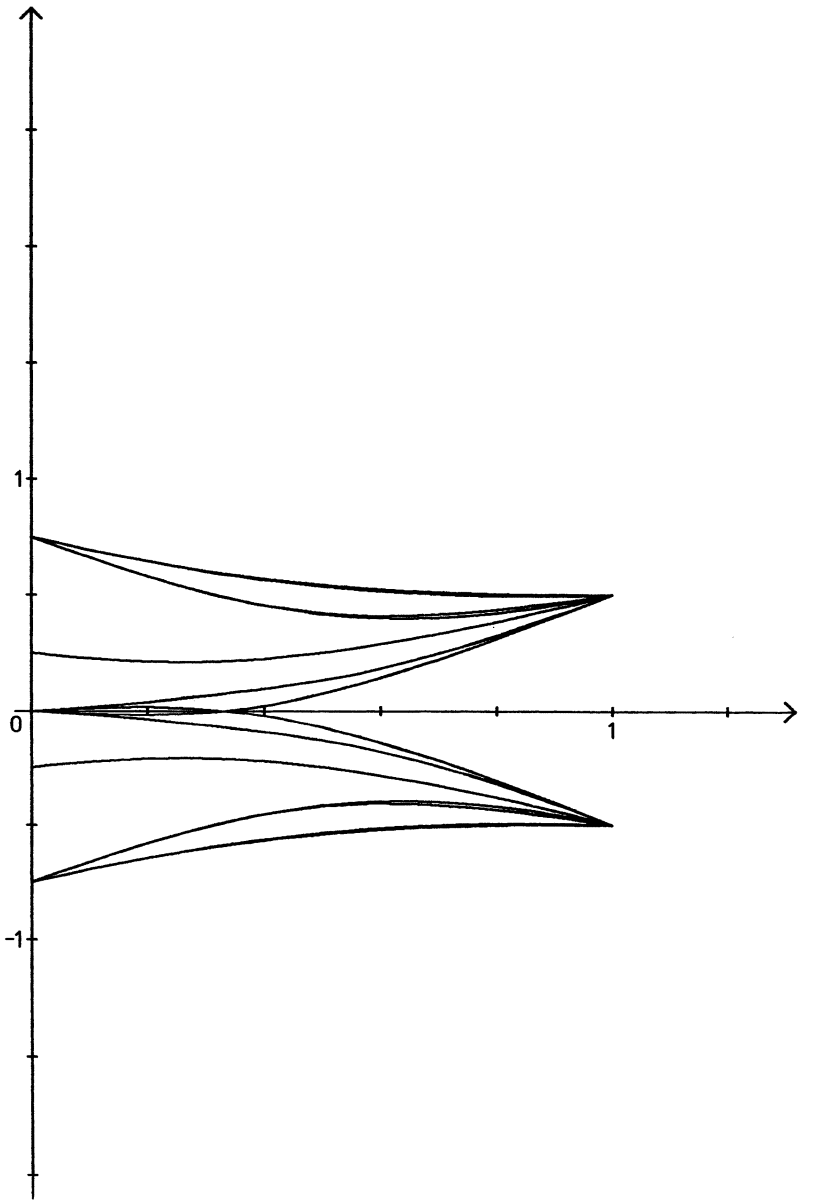

FIGURE 6. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (1, 1, 1, -1)$, $^3E_1$, in units of U-4T as a function of U.

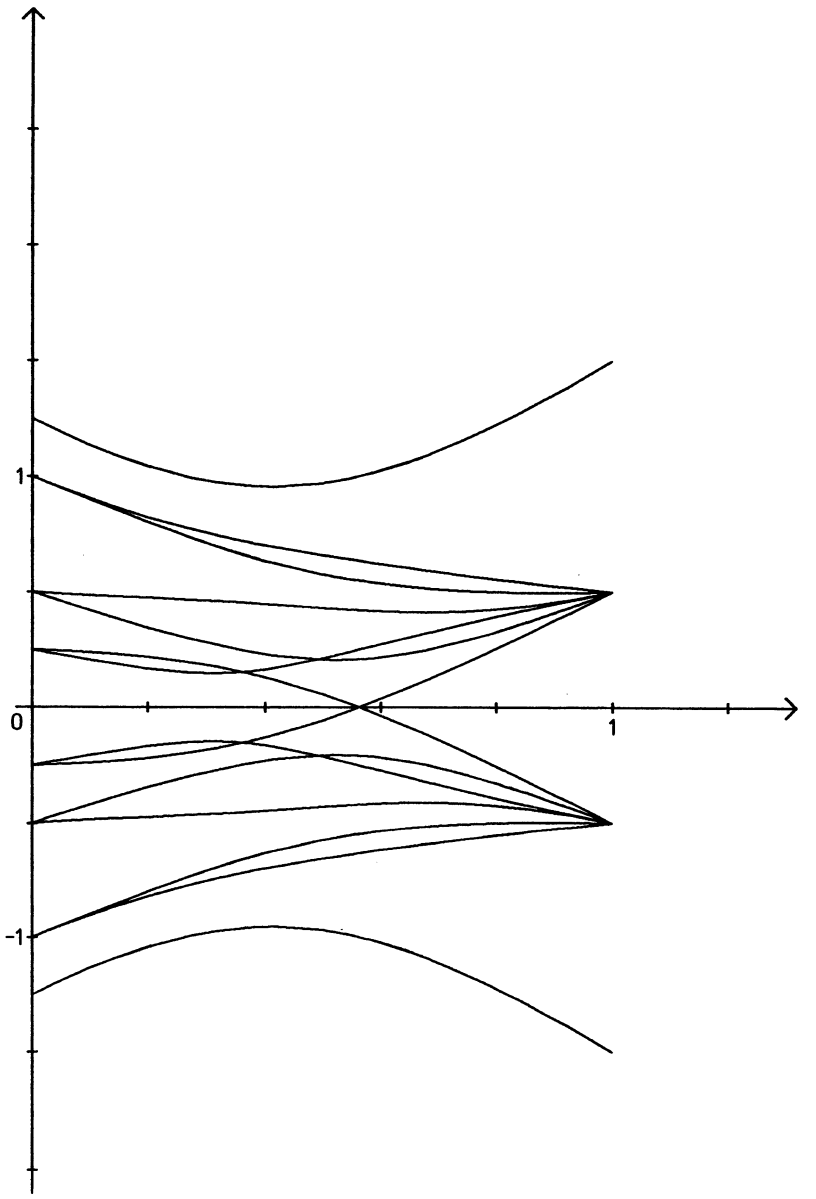

FIGURE 7. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (2, 0, 0, 1)$, $^1E_2$, in units of U-4T as a function of U.

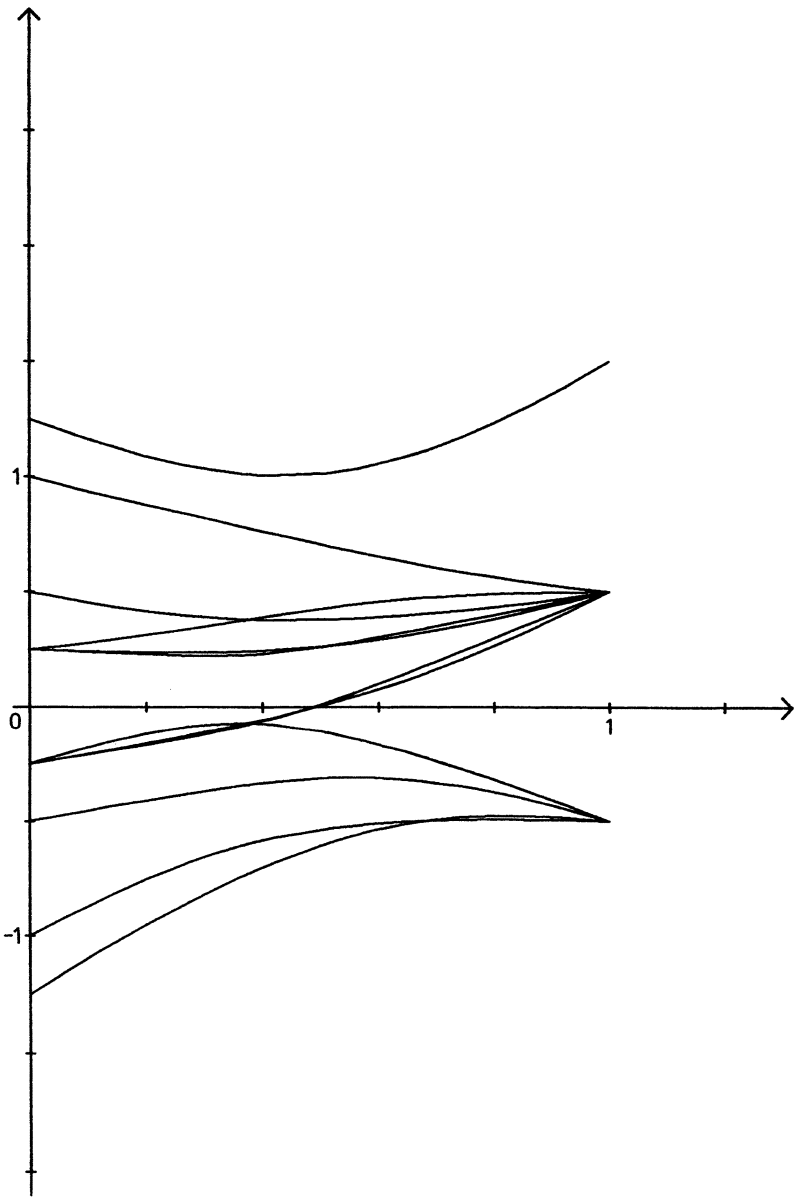

FIGURE 8. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (2, 0, 1, -1)$, $^1E_2$, in units of U-4T as a function of U. Upside down the figure shows the eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (2, 1, 0, -1)$, $^3E_2$.

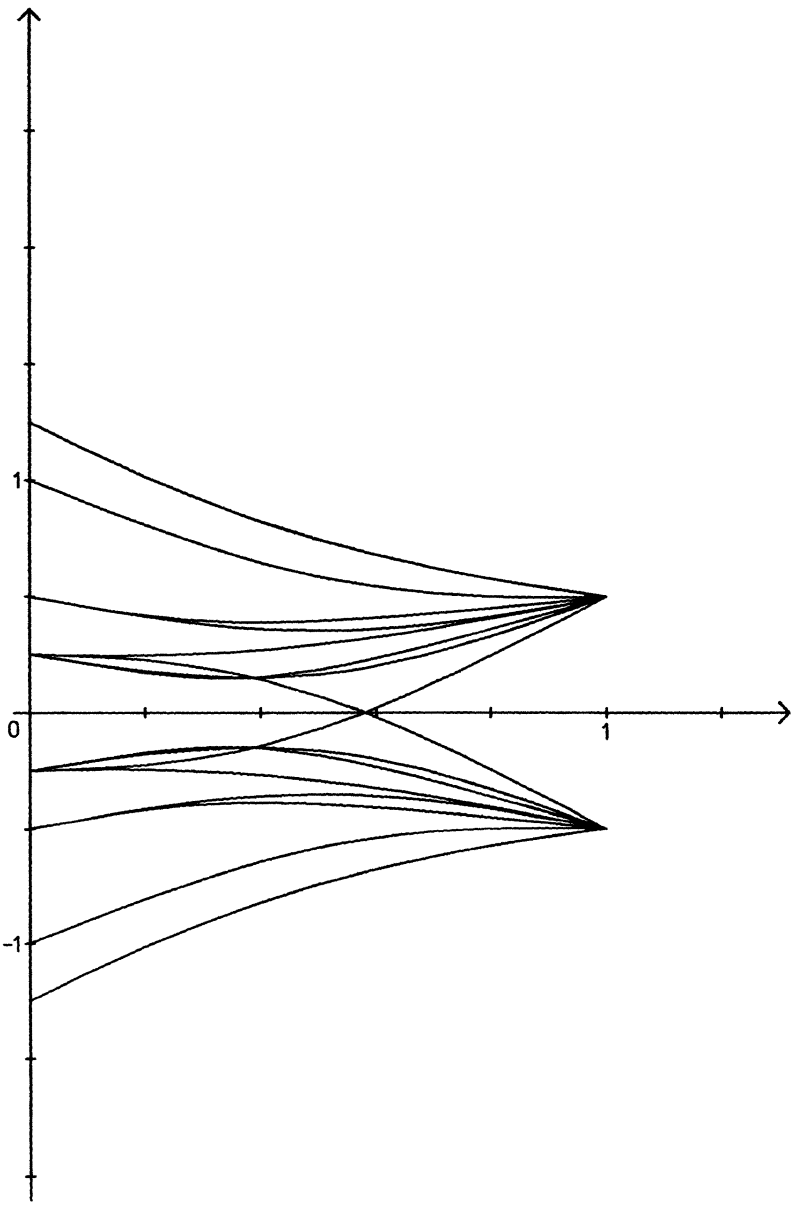

FIGURE 9. The eigenvalues for $(P, S, \hat{S}, I^{(o)}) = (2, 1, 1, 1)$, $^3E_2$, in units of U-4T as a function of U.

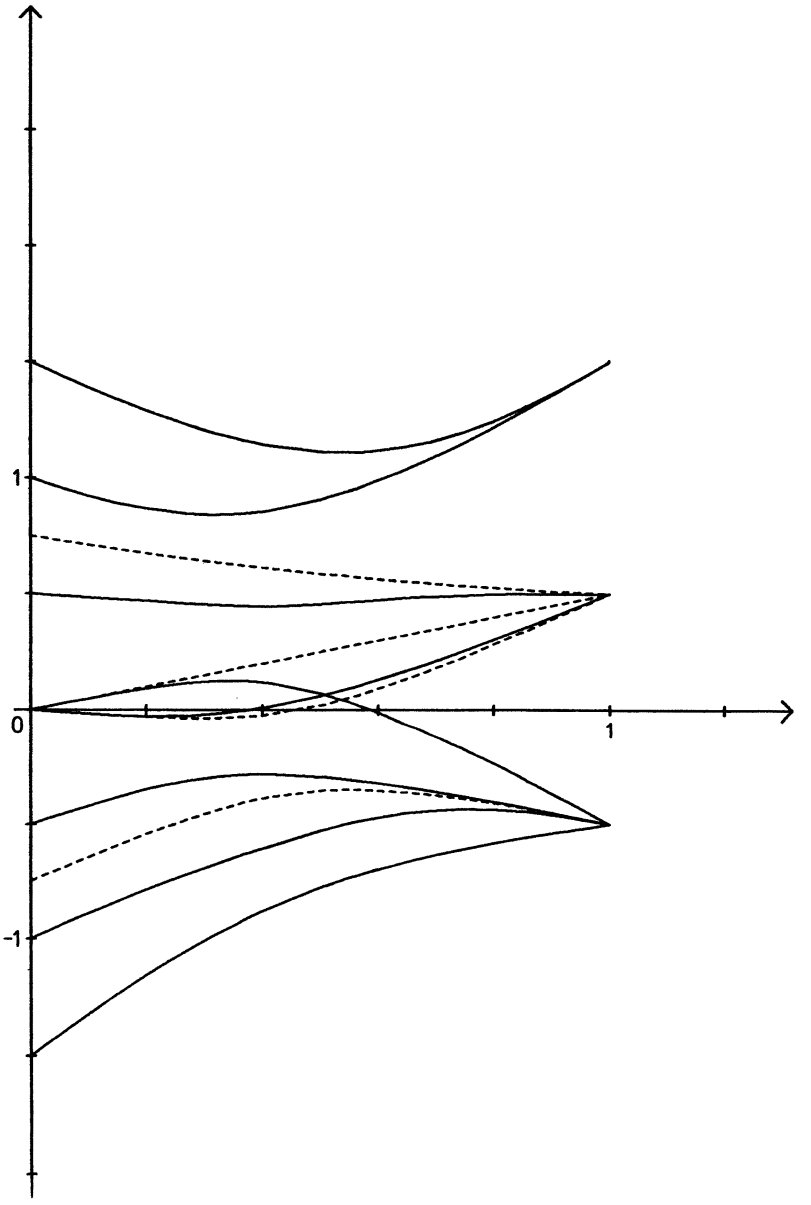

FIGURE 10. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 0, 1, -1, 1)$, $^1B_1$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 0, 1, 1, 1)$, $^1B_2$. Upside down the figure shows the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 1, 0, -1, 1)$, $^3B_1$; - - - represents in this case the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 1, 0, 1, 1)$, $^3B_2$.

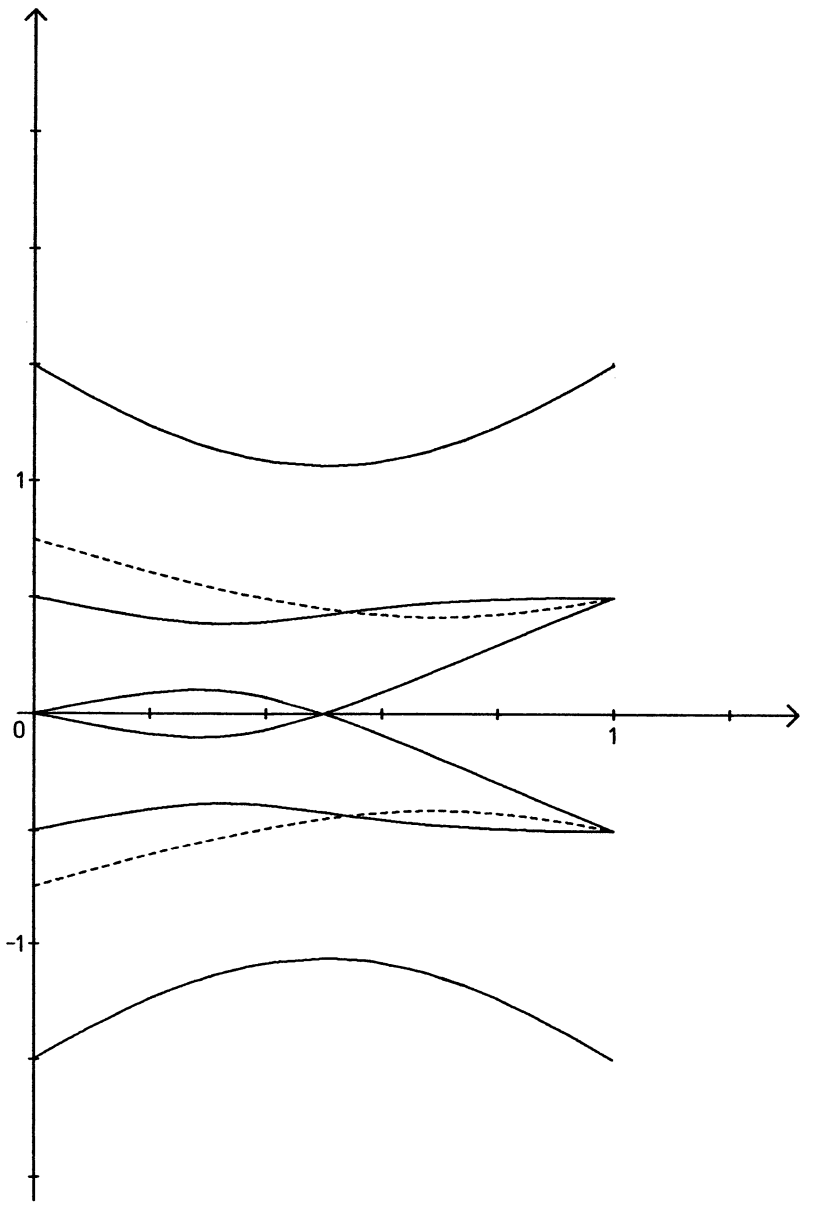

FIGURE 11. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 0, 0, 1, -1)$, $^1B_2$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 0, 0, -1, -1)$, $^1B_1$.

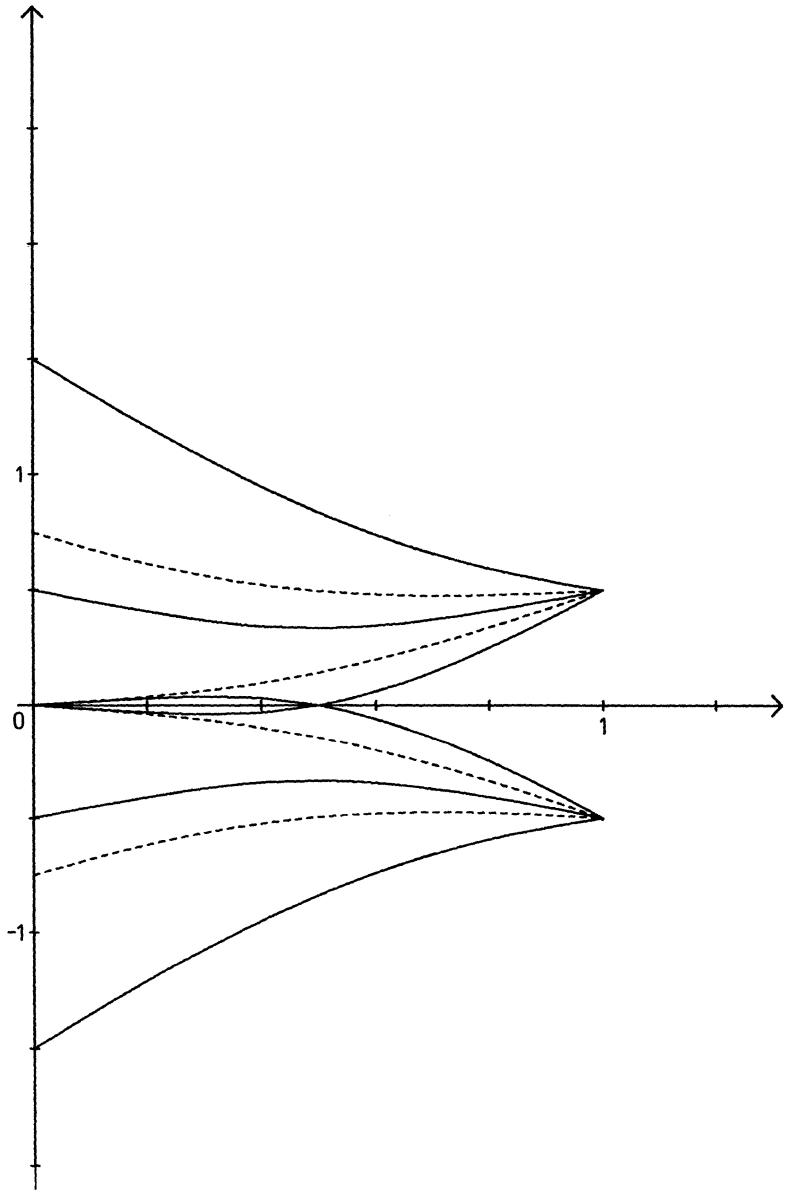

FIGURE 12. The eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 1, 1, 1, -1)$, $^3B_2$, in units of U-4T as a function of U; - - - represents also the eigenvalues for $(P, S, \hat{S}, \sigma, I^{(o)}) = (3, 1, 1, -1, -1)$, $^3B_1$.

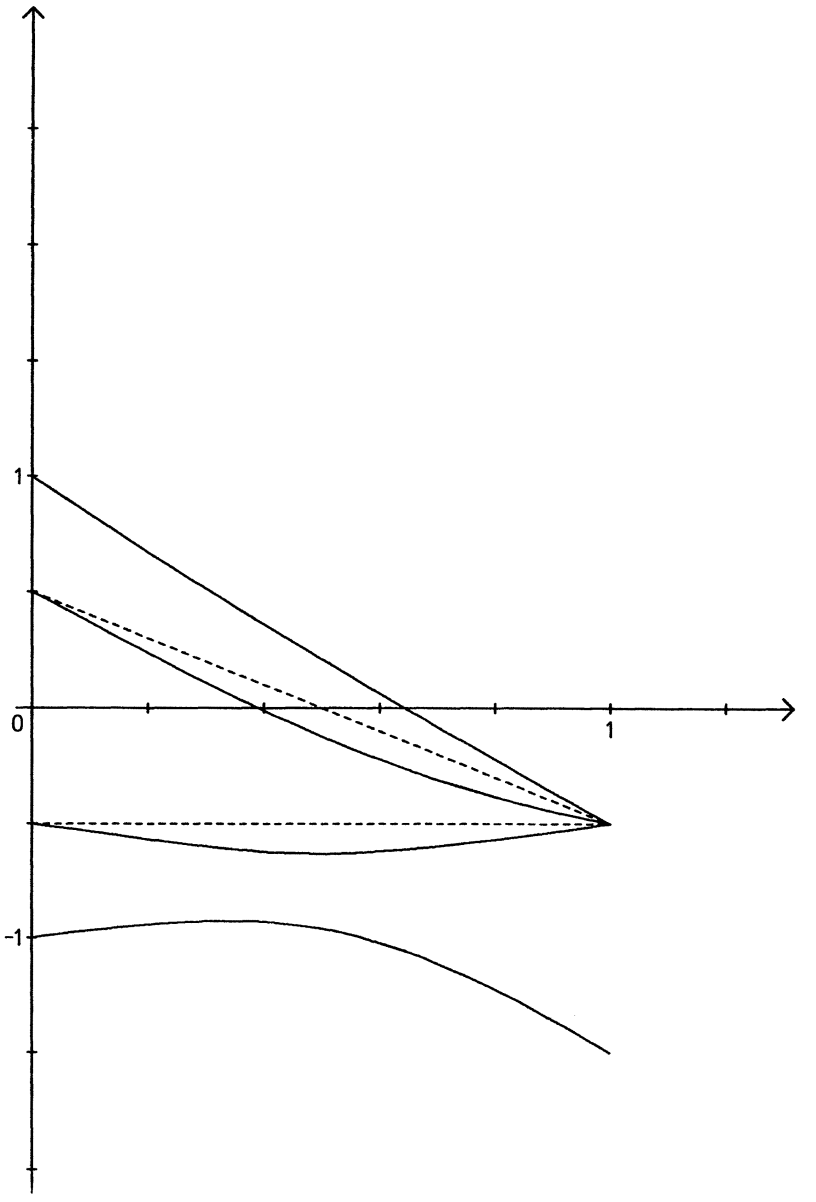

FIGURE 13. The eigenvalues for (P, S) = (0, 2) in units of U-4T as a function of U; —— corresponds to (P, S, $\hat{S}$, σ, $I^{(o)}$) = (0, 2, 0, 1, 1), $^5A_1$, and - - - corresponds to (P, S, $\hat{S}$, σ, I^o) = (0, 2, 1, −1, −1), $^5A_2$. Upside down the figure shows the eigenvalues for (P, $\hat{S}$) = (0, 2); —— corresponds then to (P, S, $\hat{S}$, σ, $I^{(o)}$) = (0, 0, 2, 1, 1), $^1A_1$ and - - - to (P, S, $\hat{S}$, σ, $I^{(o)}$) = (0, 1, 2, −1, −1), $^3A_2$.

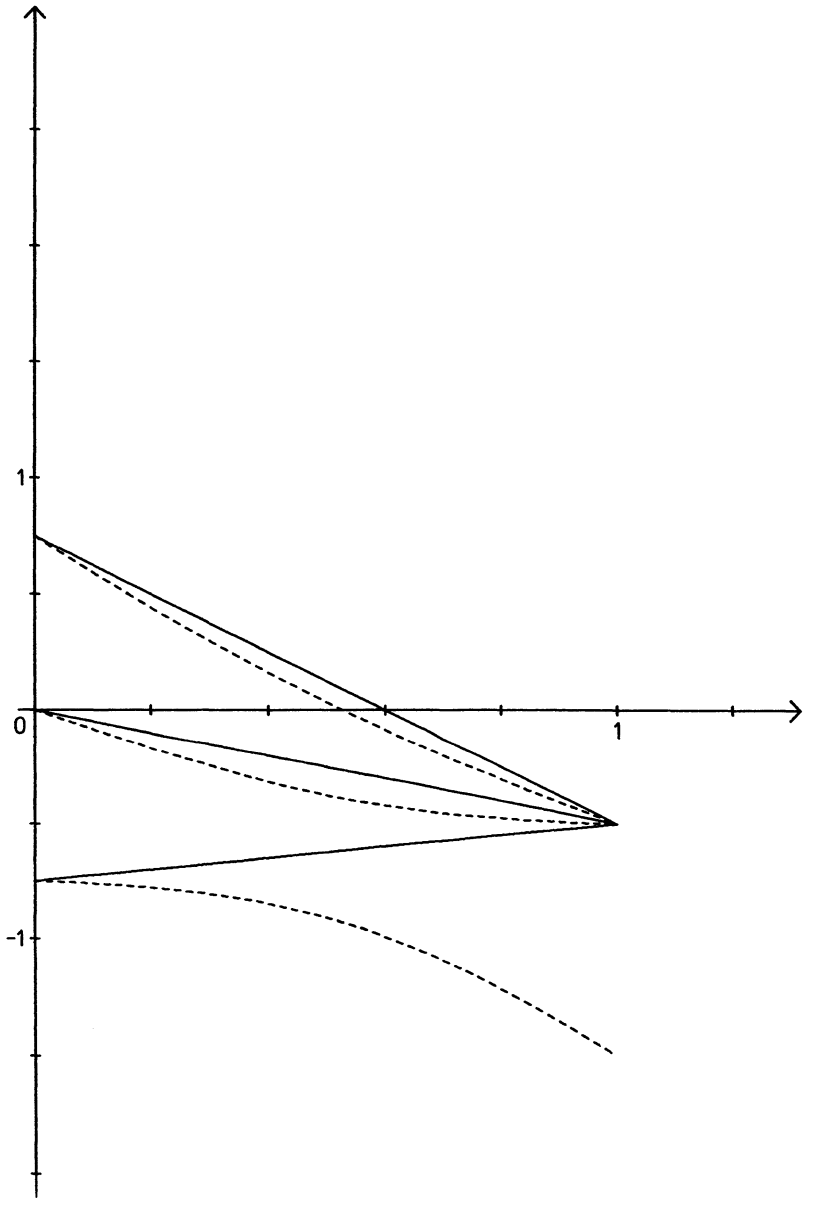

FIGURE 14. The eigenvalues for (P, S) = (1, 2) in units of U-4T as a function of U; —— corresponds to (P, S, Ŝ, $I^{(o)}$) = (1, 2, 1, 1), $^5E_1$, and --- corresponds to (P, S, Ŝ, I^o) = (1, 2, 0, −1), $^5E_1$. Upside down the figure shows the eigenvalues for (P, Ŝ) = (1, 2); —— corresponds then to (P, S, Ŝ, $I^{(o)}$) = (1, 1, 2, 1), $^3E_1$, and --- to (P, S, Ŝ, $I^{(o)}$) = (1, 0, 2, −1), $^1E_1$.

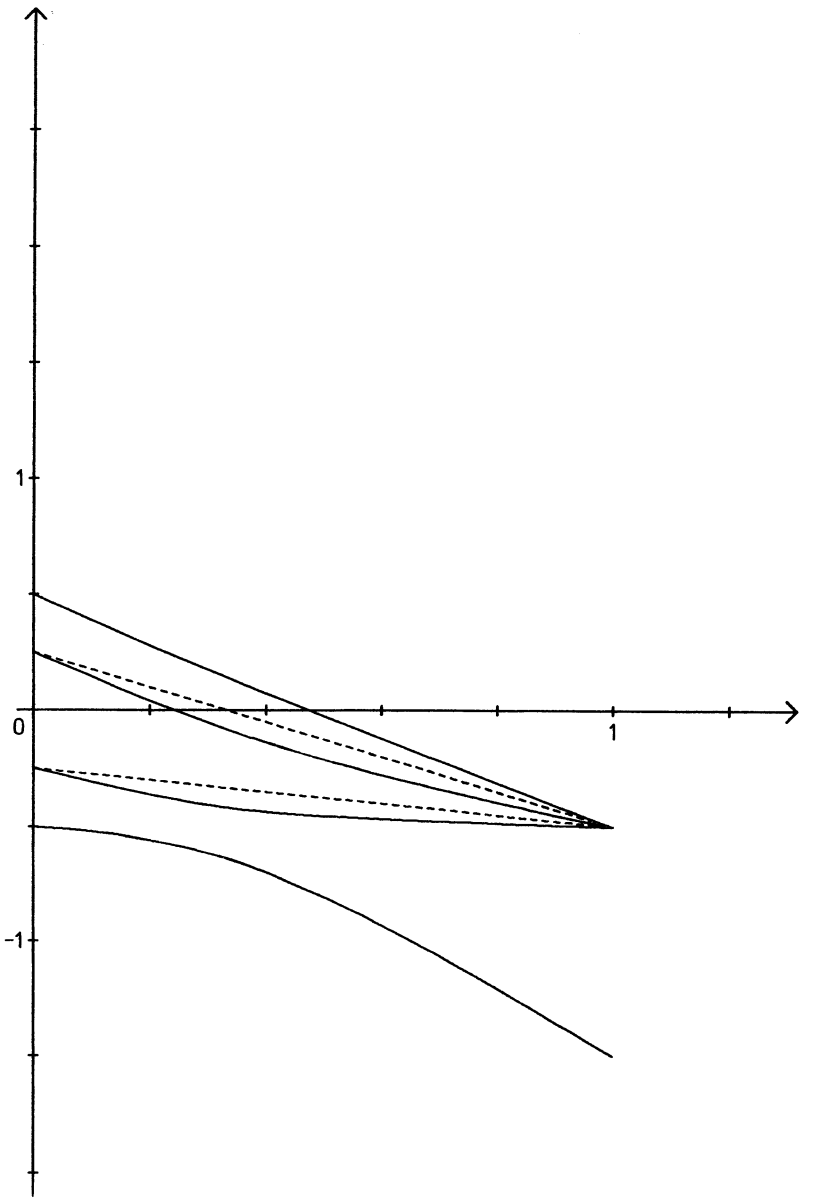

FIGURE 15. The eigenvalues for (P, S) = (2, 2) in units of U-4T as a function of U, —— corresponds to (P, S, $\hat{S}$, $I^{(o)}$) = (2, 2, 0, 1), $^5E_2$, and --- corresponds to (P, S, $\hat{S}$, $I^{(o)}$) = (2, 2, 1, −1), $^5E_2$. Upside down the figure shows the eigenvalues for (P, $\hat{S}$) = (2, 2); —— corresponds then to (P, S, $\hat{S}$, $I^{(o)}$) = (2, 0, 2, 1), $^1E_2$, and --- to (P, S, $\hat{S}$, $I^{(o)}$) = (2, 1, 2, −1), $^3E_2$.

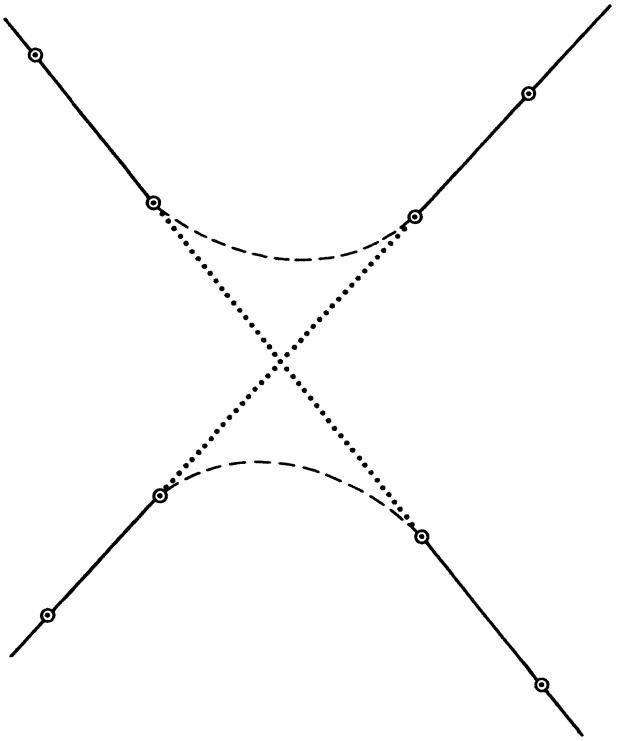

FIGURE 16. Two alternative graphs that may be drawn from given numerical data (⊙).

TABLE 2
COMPARISON AMONG EXPERIMENTS AND EXACT AND APPROXIMATE CALCULATIONS*

	Experimental†	Exact calculation‡	Exact calculation‡	Approximativ calculation§
U		6.068 eV	9.597 eV	9.597 eV
T		−2.869 eV	−3.647 eV	−3.647 eV
$^1A_1$	0	0	0	0
$^1B_2$	4.72 eV	4.72 eV	5.48 eV	
$^1B_1$	6.09 eV	7.64 eV	10.35 eV	4.81 eV
$^1E_1$	6.93 eV	7.04 eV	9.58 eV	6.77 eV
$^1E_2$		7.33 eV	8.65 eV	5.88 eV
$^3B_1$	3.66 eV	3.66 eV	4.06 eV	4.18 eV
$^3E_1$		4.68 eV	5.57 eV	5.70 eV
$^3E_2$		7.33 eV	7.45 eV	4.70 eV

*Cf. FIGURE 17.
†Quoted from G. Herzberg.[26] The symmetry assignment is due to R. Pariser.[25]
‡EQUATION 1.
§Calculated by Linderberg and Öhrn[6] by approximations to EQ. 1.

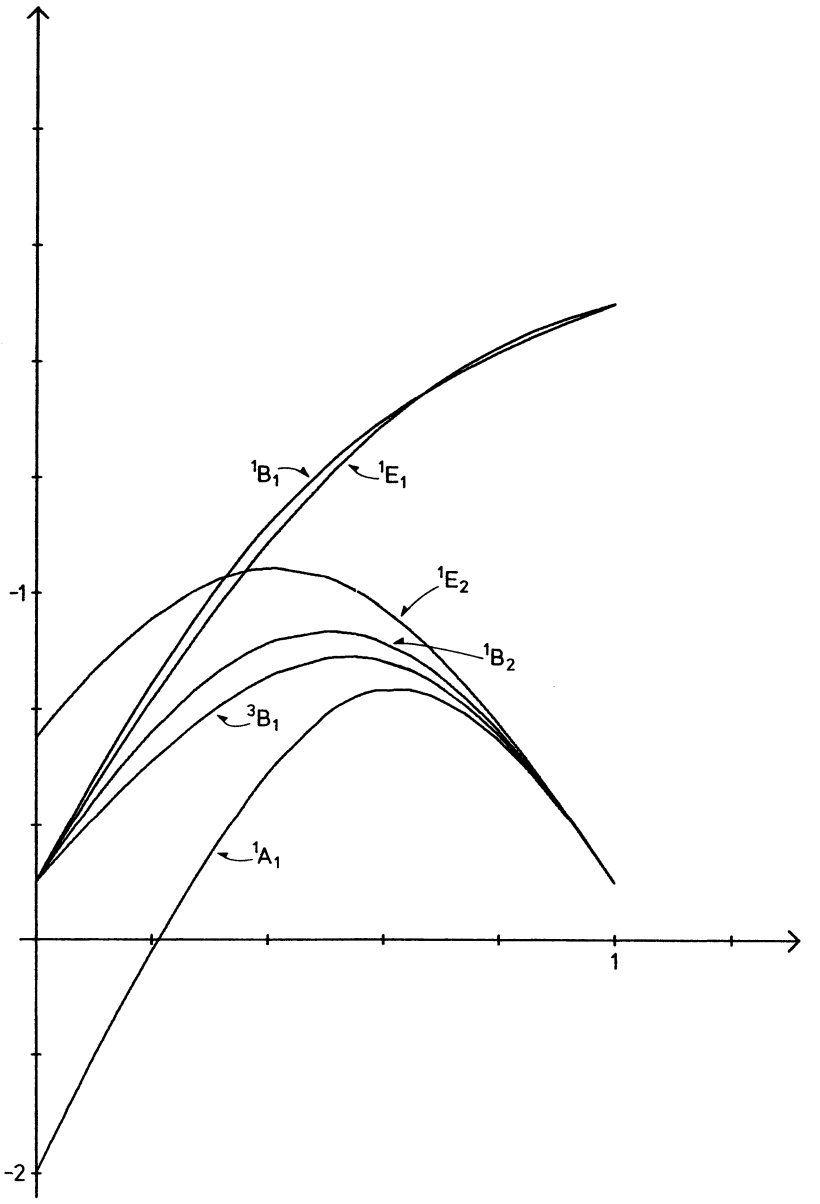

FIGURE 17. The lowest eigenvalues for $^1A_1$, $^1E_1$, $^1E_2$, $^1B_1$, $^1B_2$, and $^3B_1$ in units of U-4T as a function of U.

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gives values for $^3B_1$ and $^1B_2$ in agreement with experiment. It appears that the poor agreement between Linderberg and Öhrn's calculations[6,8] and experiment is partly due to the inadequacy of the Hubbard Hamiltonian and partly due to an inadequate approximation method.

V. The Noncrossing and Nondegeneracy Rules

The noncrossing rule was suggested by Hund[14] in 1927, and a "proof" was given by von Neumann and Wigner[15] two years later. A simplified version due to Teller[27] is the one most often quoted in textbooks.[16–20]

The rule concerns a Hamiltonian that depends on a real parameter, in our case U. All levels may be classified by symmetry quantum numbers, and the rule is that levels of the same symmetry can never cross each other as U is varied. A concommitant rule, which does not seem to have been stated explicitly but which follows from the same reasoning and the same assumptions, is the nondegeneracy rule. It states that, while energy levels of different symmetry may cross, they cannot be equal to each other for all values of U.

If these rules are believed, their violation in practice would mean that the Hamiltonian possesses a larger symmetry group than at first supposed.

The rules depend crucially on the interpretation of the word *symmetry*. The conventional meaning is that of a symmetry group independent of U; in this case the "proofs" are false. It is not difficult to construct a parameter-dependent matrix that has no symmetry yet violates both rules. If, on the other hand, one allows symmetry groups that are U-dependent, the "theorems" are mere tautologies, because it is easy to see (cf. REF. 28 for an explicit proof) that one can always invent, *post hoc*, a U-dependent symmetry group to account for any violations.

One may ask what is wrong with the "proofs" quoted above. The fault lies not in the mathematics *per se* but in the assumptions used to connect the mathematics with the real world: First, in the natural sciences, two real numbers are never equal unless there is a physical reason for it; second, that reason must be the existence of a U-independent symmetry group.

The first assumption has validity, but the second is merely a confession of ignorance in which, we hasten to add, we also share. Surely there must be a "natural" U-dependent symmetry group to account for the violations we have discovered, but we cannot find it. One thing is certain, however; all U-independent symmetry groups have been found in Section II except for minor exceptions (which are not enough to resuscitate the nondegeneracy rule) mentioned in i) and ii) below.

In order to prove that the Hubbard Hamiltonian provides a quantum mechanical counter example to the rules we will, of course, have to prove that there is no hidden symmetry. This can be done by the method described in REF. 28. The principle of the method is as follows: Finding all the U-independent symmetry of the Hamiltonian, **H**, is equivalent to finding all the U-independent invariant subspaces of **H**. If one can find a representation such that the U-independent invariant subspaces are spanned by the basic vectors for the representation then **H** becomes block-diagonal in this representation with each diagonal block corresponding to an invariant subspace. If the method is applied separately to each of the diagonal blocks into which **H** has already been split by the symmetry operators $\mathbf{C}_{2n}$, σ, $\mathbf{I}^{(o)}$ and $\mathbf{J}^{(s)}$ then one can use the simple version of the method designed for the non-degenerate case, since none of the blocks shows

permanent degeneracy. In this case, an appropriate choice of basic vectors are the eigenvectors for any value of U for which no crossing occurs. The method entails diagonalization of H and is, consequently, numerical. The results seem, however, to indicate very strongly that there is no important hidden symmetry. The known symmetry corresponding to the unused symmetry operators S^2 and $\hat{S}^2$ revealed itself even with very low numerical cutoff levels (10^{-4}). (Cutoff level refers to the criterion for declaring an off-diagonal element to be zero). Nothing else of interest showed up even with the cut-off level as high as 10^{-1}; several values of U were tried.

There is, indeed, some U-independent symmetry in addition to that given in Section II. Its significance eludes us at present, but in any case it still leaves the majority of violations unexplained. The additional U-independent symmetry is (i) For $P = 3$, $S = 2$ there is a fivefold degeneracy with $E' = U/2$, and for $P = 3$, $S = 2$ there is a fivefold degeneracy with $E' = -U/2$. For $P = 3$, $S = 1$, $\sigma = -1$, $I^{(o)} = 1$ there is an $E' = -U/2$ level, and for $P = 3$, $S = -1$, $\sigma = -1$, $I^{(o)} = 1$ there is an $E' = U/2$ level. These two groups of sixfold degenerate levels have the property that the wave functions are U-independent and hence all U-independent unitary transformations in these subspaces commute with H. (ii) For $S = 2$ or $\hat{S} = 2$, every wave function belonging to $I^{(o)} = -1$ is U-independent. The eigenvalues have no degeneracy. If one wishes, any Abelian group of operators that commutes with this subspace of H will be a U-independent symmetry group.

From the numerical point of view, the degeneracy is more interesting than the crossing: First, degeneracy definitely establishes the crossing, at least in some cases, because there are many instances where degenerate groups of levels of different symmetry cross a level of the same symmetry as one in the group. Since all levels are continuous in U, there can be no numerical ambiguity about the crossings. Second, the degeneracy is much better supported by the numerical data, as the levels are calculated for many values of U, not just one.

Even though the results of the numerical calculations render both the existence of degeneracy and the absence of hidden symmetry very probable, it would be preferrable to have a rigorous proof. It is merely a question of work to prove the degeneracy, since this can be done by evaluating the characteristic polynomials for the respective matrices in closed form and then prove one polynomial to be a factor in the other. To prove the nonexistence of additional symmetry one would in general need a complicated error analysis. However, it is very fortunately the case that if one choses the subspaces ($P = 3$, S even, $\sigma = 1$, $I^{(o)} = 1$) and ($P = 3$, S even, $\sigma = -1$, $I^{(o)} = 1$) then it is possible to apply the general method of REF. 28 in such a manner that one has to diagonalize only 2×2 matrices. The submatrices of H that correspond to the two chosen subspaces are shown in TABLES 3 and 4.

For $\sigma = 1$ (TABLE 3), there are no problems. States no. 2 and no. 3 with eigenvalues U/2 and $-U/2$ correspond to $(S, \hat{S})$ equal to (0, 2) and (2, 0), respectively. The remaining two levels correspond to $(S, \hat{S}) = (0, 0)$ with energies

$$E' = \pm (9T^2 + \tfrac{1}{4}U^2)^{\frac{1}{2}}. \tag{79}$$

For $\sigma = -1$ (TABLE 4), we apply the method of REF. 28 to find the symmetry.

By choosing $U = 0$ we can use the fact that the T-part is already diagonal. The energy levels 6T, 3T, 2T, $-2T$, $-3T$, and $-6T$ are all nondegenerate, and the only freedom left concerns the choice of basic vectors for the eigenspace

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TABLE 3*
ONE SUBMATRIX OF H'

Wave Function No.	T-Part	U-Part			
1	−3	0	0	0	3
2	0	0	3	0	0
3	0	0	0	−3	0
4	3	3	0	0	0

*The T-part and U-part of the submatrix of H' that corresponds to $P = 3$, S even, $\sigma = 1$, and $I^{(o)} = 1$. The numbering of the wave functions is arbitrary. Since the T-part is diagonal, only the diagonal is shown. The U-part should be multiplied by 1/6.

corresponding to the fourfold degenerate level 0. These vectors are fixed such that the U-part becomes block-diagonal as far as possible.

TABLE 4
ONE SUBMATRIX OF H'

Wave Function No.	T-Part	U-Part								
1	−6	0	0	1	−1	$\sqrt{18}$	$-\sqrt{2}$	$-\sqrt{2}$	0	−1	0
2	−2	0	0	−1	1	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	0	0	−1
3	0	1	−1	1	0	$-\sqrt{2}$	$\sqrt{8}$	0	$-\sqrt{2}$	−1	1
4	0	−1	1	0	−1	$-\sqrt{2}$	0	$\sqrt{8}$	$\sqrt{2}$	−1	1
5	−3	$\sqrt{18}$	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	0	2	−2	−3	0	0
6	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{8}$	0	2	−1	0	2	$\sqrt{2}$	$-\sqrt{2}$
7	0	$-\sqrt{2}$	$\sqrt{2}$	0	$\sqrt{8}$	−2	0	1	2	$-\sqrt{2}$	$\sqrt{2}$
8	3	0	0	$-\sqrt{2}$	$\sqrt{2}$	−3	2	2	0	$\sqrt{2}$	$\sqrt{18}$
9	2	−1	0	−1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	0	0
10	6	0	−1	1	1	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{18}$	0	0

*The T-part and U-part of the submatrix of H' that corresponds to $P = 3$, S even, $\sigma = -1$, and $I^{(o)} = 1$. The numbering of the wave functions is arbitrary. Since the T-part is diagonal, only the diagonal is shown. The U-part should be multiplied by 1/6.

According to the method, we start by diagonalizing the submatrix of the U-part that involves only the four states with zero eigenvalue of T. The submatrix is:

$$\begin{array}{c} (3) \\ (4) \\ (6) \\ (7) \end{array} \begin{Bmatrix} 1 & 0 & \sqrt{8} & 0 \\ 0 & -1 & 0 & \sqrt{8} \\ \sqrt{8} & 0 & -1 & 0 \\ 0 & \sqrt{8} & 0 & 1 \end{Bmatrix} \tag{80}$$

(The number of the respective wave functions are listed at the left.) Transformation to the new basic set:

$$\begin{aligned}(3A) &= \sqrt{2/3}\,(3) + \sqrt{1/3}\,(6)\\ (6A) &= \sqrt{1/3}\,(3) - \sqrt{2/3}\,(6)\\ (4A) &= \sqrt{2/3}\,(7) + \sqrt{1/3}\,(4)\\ (7A) &= \sqrt{1/3}\,(7) - \sqrt{2/3}\,(4)\end{aligned} \tag{81}$$

obviously makes EQ. 80 diagonal. The new matrix for $\sigma = -1$ is given in TABLE 5 and FIGURE 18. The functions 3A and 4A can still be rotated, since 3A and 4A have the same diagonal element after the diagonalization of EQ. 80. Next, we consider the intersection between state 1 and states 3A and 4A,

$$\begin{matrix}(3A)\\(4A)\end{matrix}\quad\begin{Bmatrix}0\\-\sqrt{3}\end{Bmatrix}, \tag{82}$$

and we see that the matrix (EQ. 82) is already in a form with as many zeros as possible and that no further rotation of 3A, 4A will produce more zeroes. By a similar argument, we find that 6A, 7A should also not be rotated further. The graph that represents the connectedness of the matrix is shown in Fig. 18.

The states 3A and 7A with energies U/2 and −U/2 correspond to S, $\hat{S}$ equal to (0,2) and to (2,0), respectively. The other eight states are connected in the graph, and, according to REF. 28, there can be no further symmetry.

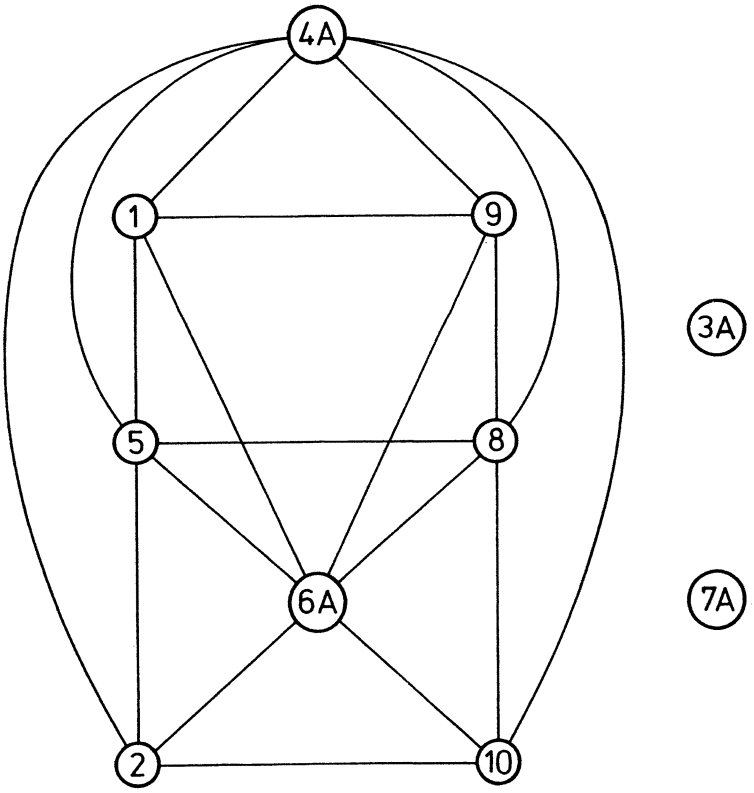

FIGURE 18. The graph of the matrix given in TABLE 5.

TABLE 5*
ONE SUBMATRIX OF H'

Wave Function No.	T-Part	U-Part								
1	-6	0	0	$\sqrt{18}$	0	$\sqrt{3}$	0	$-\sqrt{3}$	0	-1	0
2	-2	0	0	$\sqrt{2}$	0	$-\sqrt{3}$	0	$\sqrt{3}$	0	0	-1
5	-3	$\sqrt{18}$	$\sqrt{2}$	0	0	$-\sqrt{6}$	0	$-\sqrt{6}$	-3	0	0
3A	0	0	0	0	3	0	0	0	0	0	0
6A	0	$\sqrt{3}$	$-\sqrt{3}$	$-\sqrt{6}$	0	-3	0	0	$-\sqrt{6}$	$-\sqrt{3}$	$\sqrt{3}$
7A	0	0	0	0	0	0	-3	0	0	0	0
4A	0	$-\sqrt{3}$	$\sqrt{3}$	$-\sqrt{6}$	0	0	0	3	$\sqrt{6}$	$-\sqrt{3}$	$\sqrt{3}$
8	3	0	0	3	0	$-\sqrt{6}$	0	$\sqrt{6}$	0	$\sqrt{2}$	$\sqrt{18}$
9	2	-1	0	0	0	$-\sqrt{3}$	0	$-\sqrt{3}$	$\sqrt{2}$	0	0
10	6	0	-1	0	0	$\sqrt{3}$	0	$\sqrt{3}$	$\sqrt{18}$	0	0

The submatrix of H' that corresponds to P = 3, S even, $\sigma = -1$ and $I^{(o)} = 1$ after the transformation given in EQ. 81. Again, the U-part should be multiplied by 1/6.

By using a computer it is possible to evaluate the characteristic polynomial of the matrix in TABLE 5 in closed form. Eliminating the two known roots, U/2 and $-$U/2, one gets the following eighth-order polynomial ($U' = U/6$);

$$x^8 + (-49T^2 - 108\,U'^2)\,x^6 + (504T^4 + 2115\,U'^2\,T^2 + 2430\,U'^4)\,x^4 + (-1296T^6 - 10368U'^2T^4 - 15795\,U'^4\,T^2 - 20412U'^6)\,x^2 + 11664U'^2\,T^6 - 40824U'^4\,T^4 + 6561U'^6\,T^2 + 59049U'^8, \quad (83)$$

By showing that the polynomial

$$x^2 - (9T^2 + 9U'^2) \quad (84)$$

is a factor in the eighth-order polynomial, we will have shown that the eigenvalues for P = 3, S = 0, $\hat{S} = 0$, $\sigma = 1$, $I^{(o)} = 1$ as given by EQ. 79 are in fact also eigenvalues for P = 3, S = 0, $\hat{S} = 0$, $\sigma = -1$, $I^{(o)} = -1$. This can be shown to be true by synthetic division by the polynomial (EQ. 84), thereby concluding the proof of the degeneracy.

APPENDIX: IMPLICATIONS OF CERTAIN KINDS OF "PSEUDOSYMMETRY"

Here we gather together some important but far from novel formulas that are needed in the text.

It is well known that symmetry of a Hermitian operator, H, corresponds to the existence of unitary operators, A_1, A_2 · · · , which commute with H:

$$A_j H - H A_j = 0, \; (j = 1, 2, \cdots) . \quad (A.1)$$

The implication of EQ. A.1 is the possibility of diagonalizing A_j and H simultaneously, and, if some of the A_j's do not commute, this might imply degeneracy of the eigenvalues of H. We shall now study the implications of other equations that formally resemble (A.1).

The first of these is the anticommutation relation

$$BH + HB = 0 , \quad (A.2)$$

with B nonsingular. If Ψ is an eigenstate of H with eigenvalue ϵ, then

$$\mathbf{H}\Psi = \epsilon\Psi \,. \tag{A.3}$$

EQUATION A.2 implies that $\mathbf{B}\Psi$ is an eigenstate of H with eigenvalue $-\epsilon$:

$$\mathbf{HB}\Psi = -\epsilon\mathbf{B}\Psi \tag{A.4}$$

and the nonzero eigenvalues of H occur in pairs with opposite sign. If EQ. A.1 and A.2 are taken together, one gets

$$(\mathbf{B}^{-1}\mathbf{A}_j\mathbf{B})\mathbf{H} - \mathbf{H}(\mathbf{B}^{-1}\mathbf{A}_j\mathbf{B}) = 0 \tag{A.5}$$

which implies that the mapping:

$$\mathbf{A}_j \rightarrow \mathbf{B}^{-1}\ \mathbf{A}_j\ \mathbf{B} \tag{A.6}$$

is a 1:1 mapping of the set of all operators that commute with H onto itself. Furthermore, the mapping

$$\mathbf{A}_j \rightarrow \mathbf{B}\ \mathbf{A}_j \tag{A.7}$$

is a 1:1 mapping of the set of all operators that commute with H onto the set of all operators, which anticommute with H. Conclusion: To find the entire set of anticommuting operators it is necessary to know only one of them, together with the entire set of commuting operators.

Next we shall consider a generalized commutation relation:

$$\mathbf{C}\ \mathbf{H} - \mathbf{H}\ \mathbf{C} = \mathbf{C}\ \mathbf{K} \tag{A.8}$$

with the following constraint on K:

$$\mathbf{H}\ \mathbf{K}\ - \mathbf{K}\ \mathbf{H} = 0 \tag{A.9}$$

If Ψ is simultaneously an eigenstate of H with eigenvalue ϵ and of K with eigenvalue κ (this is possible according to EQ. A.9), then one has

$$\mathbf{H}\ \mathbf{C}\ \Psi = (\epsilon - \kappa)\mathbf{C}\ \Psi \,. \tag{A.10}$$

If, further, C and K anticommute:

$$\mathbf{C}\ \mathbf{K} + \mathbf{K}\ \mathbf{C} = 0 \,, \tag{A.11}$$

then we have EQ. A.4 again:

$$\mathbf{K}\ \mathbf{C}\ \Psi = -\kappa\ \mathbf{C}\Psi \,. \tag{A.12}$$

Another trivial consequence of EQ. A.8, A.9, and A.11 is that

$$\mathbf{C}^2\ \mathbf{H} - \mathbf{H}\ \mathbf{C}^2 = 0 \,. \tag{A.13}$$

Actually, the conditions A.13 and A.11 are equivalent when A.8 and A.9 obtain.

If, in addition, C is nonsingular, the mapping

$$\mathbf{A}_j \rightarrow \mathbf{C}^{-1}\ \mathbf{A}_j\ \mathbf{C} \tag{A.14}$$

will be a 1:1 mapping of the set of operators that commute with both K and H onto itself.

Finally, we shall consider a generalized anticommutator relation:

$$\begin{aligned} &\mathbf{D}\ \mathbf{H} + \mathbf{H}\ \mathbf{D} = \mathbf{D}\ \mathbf{L} \\ &\mathbf{H}\ \mathbf{L} - \mathbf{L}\ \mathbf{H} = 0 \,. \end{aligned} \tag{A.15}$$

If Ψ is simultaneously an eigenstate of H with eigenvalue ϵ and of L with eigenvalue λ, then one has

$$\mathbf{H}\ \mathbf{D}\ \Psi = (\lambda - \epsilon)\mathbf{D}\ \Psi\ . \tag{A.16}$$

If, further, D and L commute:

$$\mathbf{D}\ \mathbf{L} - \mathbf{L}\ \mathbf{D} = 0 \tag{A.17}$$

then one has:

$$\mathbf{L}\ \mathbf{D}\ \Psi = \lambda\ \mathbf{D}\ \Psi \tag{A.18}$$

and

$$\mathbf{D}^2\ \mathbf{H} - \mathbf{H}\ \mathbf{D}^2 = 0\ . \tag{A.19}$$

If D is nonsingular, the mapping

$$\mathbf{A}_j \rightarrow \mathbf{D}^{-1}\ \mathbf{A}_j\ \mathbf{D} \tag{A.20}$$

is a 1:1 map of the set of operators, which commute with both L and H, onto itself.

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Two Theorems on the Hubbard Model

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In the attractive Hubbard model (and some extended versions of it), the ground state is proved to have spin angular momentum $S=0$ for every (even) electron filling. In the repulsive case, and with a bipartite lattice and a half-filled band, the ground state has $S=\frac{1}{2}||B|-|A||$, where $|B|$ ($|A|$) is the number of sites in the B (A) sublattice. In both cases the ground state is unique. The second theorem confirms an old, unproved conjecture in the $|B|=|A|$ case and yields, with $|B|\neq|A|$, the first provable example of itinerant-electron ferromagnetism. The theorems hold in all dimensions without even the necessity of a periodic lattice structure.

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The importance of the Hubbard model of itinerant electrons is increasingly being appreciated. Because of the model's subtlety, rigorous results and exact solutions are clearly useful bench marks, but these are rare. Two theorems about the ground states are stated and proved here. Parts of them are resolutions of old conjectures while other parts are new. In particular, the assertion that certain versions of the model show ferromagnetic behavior for the half-filled band is, I believe, new and yields the first provable example of itinerant-electron ferromagnetism with finite forces and without *ad hoc* assumptions.

After some preliminary definitions, the two theorems are stated. Each is followed by some remarks about their significance. Finally, the proofs are given. The proofs utilize a new kind of reflection positivity which does not involve the usual spatial reflections but rather reflections in spin space. In fact, spatial symmetry plays no role whatsoever and therefore the theorems apply in the widest generality to any collection of sites; all dimensions and topologies are included. The Hubbard model is not known to satisfy any kind of spatial reflection positivity or infrared bounds and this unfortunate fact has prevented the application of the usual proof techniques[1–3] for establishing the existence of long-range order in periodic lattices.

The Hubbard model on a finite lattice Λ is defined by the Hamiltonian

$$H=\sum_{\sigma}\sum_{x,y\in\Lambda}t_{xy}c^{\dagger}_{x\sigma}c_{y\sigma}+\sum_{x\in\Lambda}U_x n_{x\uparrow}n_{x\downarrow}\,, \tag{1}$$

with the following notation. The operators $c_{x\uparrow}$ and $c_{x\downarrow}$ and their adjoints $c^{\dagger}_{x\sigma}$ satisfy the usual fermion anticommutation relations $\{c^{\dagger}_{x\sigma},c_{y\tau}\}=\delta_{xy}\delta_{\sigma\tau}$ and $\{c_{x\sigma},c_{y\tau}\}=0$. The hopping matrix elements t_{xy} are required to be real and satisfy $t_{xy}=t_{yx}$, but no other *a priori* assumption is made about them (e.g., the condition $t_{xx}=0$ is not assumed, which means that an x-dependent single-particle potential $\sum_{x\sigma}t_{xx}n_{x\sigma}$ is allowed). The reality of the t_{xy}'s is consistent with their interpretation as overlap matrix elements of real operators in real, localized orbitals. The number operators are $n_{x\sigma}=c^{\dagger}_{x\sigma}c_{x\sigma}$, while U_x is the on-site energy which, for theorem 1, is allowed to depend on the site x. The word "lattice" is certainly a misnomer because no particular topology (i.e., periodicity or dimensionality) is assumed; the generality assumed here is that Λ is merely a collection of sites. The number of these sites is denoted by $|\Lambda|$. There is said to be a *bond* between sites x and y if $t_{xy}\neq0$, and Λ is said to be *connected* if there is a connected path of bonds between every pair of sites. Obviously it is no loss in generality to assume that Λ is connected, and this will always be done here. Finally, Λ is said to be *bipartite* if the sites of Λ can be divided into two disjoint sets A and B such that $t_{xy}=0$ whenever $x\in A$ and $y\in A$ or $x\in B$ and $y\in B$. The bipartite condition is really an assertion about the t_{xy}'s and not about Λ, but the terminology is conventional; it implies, in particular, that $t_{xx}=0$ for each $x\in\Lambda$. The symbols $|A|$ and $|B|$ denote the number of sites in A and B in this case, whence $|\Lambda|=|A|+|B|$. The number of electrons is denoted by N; necessarily $N\leq2|\Lambda|$.

The aim here is to study the ground state (or states if there is more than one) of H for a given N. Of central importance is the total spin S which is a conserved quantity. The spin operators are the quadratic operators

$$S^z=\tfrac{1}{2}\sum_{x\in\Lambda}(n_{x\uparrow}-n_{x\downarrow}),\ S^+=(S^-)^{\dagger}=\sum_{x\in\Lambda}c^{\dagger}_{x\uparrow}c_{x\downarrow}\,, \tag{2}$$

and $(S_{\rm op})^2=(S^z)^2+\frac{1}{2}S^+S^-+\frac{1}{2}S^-S^+$, with eigenvalues $S(S+1)$.

Theorem 1 (attractive case).—Assume $U_x\leq0$ for every x (but U_x is not necessarily constant) and that N is even. No extra assumption about Λ or the t_{xy}'s is made. Then (a) among the ground states of H there is one with spin $S=0$; (b) if $U_x<0$ for every x, the ground state is unique (and hence has $S=0$).

Remarks.—(1) The theorem is "obvious" if all the U_x's are very large, for then the ground state consists of paired electrons on $N/2$ sites of Λ. In the other extreme that each $U_x=0$, theorem 1 is also obvious because one just fills the lowest $N/2$ levels of the $|\Lambda|\times|\Lambda|$ Hermi-

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tian hopping matrix $T=\{t_{xy}\}$.

(2) Theorem 1 can be considerably generalized to what is called an *extended Hubbard model,* and more. We can add any *real* operator M to H provided that M satisfies the following two conditions. (A real operator is polynomial in the $c_{x\sigma}$'s and $c_{x\sigma}^{\dagger}$'s with real coefficients.) (i) M commutes with the spin operators S^z and $S^{\pm}$ and conserves both spin-up and spin-down particle numbers; (ii) M can be written as $M^{\uparrow}+M^{\downarrow}-M^{\uparrow\downarrow}$. Here $M^{\uparrow}$ ($M^{\downarrow}$) is real, Hermitian, involves only spin-up (spin-down) operators, and $M^{\uparrow}$ is identical to $M^{\downarrow}$ when the spins are flipped (i.e., $c_{x\uparrow}$ and $c_{x\downarrow}$ are interchanged). The up-down interaction $M^{\uparrow\downarrow}$ can be written as a sum of terms of the form (in which μ merely denotes a summation index) $M^{\uparrow\downarrow}=\sum_{\mu}V_{\mu}^{\uparrow}(V_{\mu}^{\downarrow})^{\dagger}$ in which each V_{μ} operator is real (but not necessarily Hermitian) and involves only operators for one kind of electron. Again, $V_{\mu}^{\uparrow}$ must be the spin reflection of $V_{\mu}^{\downarrow}$ for each μ. The necessary changes in the proof are straightforward (see Ref. 4). It is also easy to extend the proof to some multiband Hubbard models; the details are left to the reader.

Theorem 2 (repulsive case).—Assume $U_x=U$ =positive constant, independent of x. Assume $|\Lambda|$ is even, Λ is bipartite (so that the t_{xy}'s couple only A and B) and $|B|\geq|A|$. No other assumption about Λ or the t_{xy}'s is made. Let $N=|\Lambda|$ (half-filled band). Then the ground state of H is unique [apart from the trivial $(2S+1)$-fold degeneracy] and has spin $S=\frac{1}{2}\times(|B|-|A|)$.

Remarks.—(3) Theorem 2 is considerably more subtle than theorem 1. The assumptions are more stringent. The theorem has long been assumed to be true in the $|B|=|A|$ case ("the half-filled band has spin zero"), but its proof has been elusive.

(4) The fact that $2S=|B|-|A|$ should be no surprise. In the limit $U=0$ we fill the levels of the matrix $T=\{t_{xy}\}$ and one might hastily conclude that S must be zero in this limit. If so, theorem 2 would be contradicted by a continuity argument with respect to U. However, the rank of T is at most $2|A|$ and so T has at least $|\Lambda|-2|A|=|B|-|A|$ zero eigenvalues. The remaining eigenvalues of T come in plus-minus pairs, so that T has at most $|A|$ negative eigenvalues. To achieve $2S=|B|-|A|$, we fill the negative levels twice with opposite spins and place the remaining electrons in the zero levels with a common spin, say, spin up. Thus the ground state is degenerate when $U=0$, but $S=\frac{1}{2}(|B|-|A|)$ is among them. Therefore, there is no contradiction with the continuity argument mentioned above. If, on the other hand, U is very large we know[5] from second-order perturbation theory that H is effectively an isotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnet with Hamiltonian

$$h=(2/U)\sum_{x,y}t_{xy}^{2}(\mathbf{S}_x\cdot\mathbf{S}_y-\tfrac{1}{4}).$$

For such models it is also known[6] that the ground state is unique and has $2S=|B|-|A|$.

(5) It is easy to construct many regular, periodic lattices in every dimension greater than one with $|B|\neq|A|$. A classic (high-T_c superconductor) two-dimensional example is to start with a square lattice and then intercalate one site in the middle of each bond. The original vertices of the squares are A sites (copper) and the intercalated sites are B sites (oxygen). The half-filled band has three electrons per unit cell and theorem 2 says that then the total net magnetization is $S=\frac{1}{2}(2-1)=\frac{1}{2}$ times the number of unit cells. This was already observed for this lattice in the large-U limit by Mattis.[7]

Whether or not this example is physically realizable is less important than the fact that theorem 2 applied to a periodic lattice with $|B|>|A|$ yields, for the first time, a natural, provable example of an *itinerant-electron model of ferromagnetism.* I use the word ferromagnetism here only in the sense that the spin is extensive, i.e., it is proportional to the number of particles (or cells). Spatial ordering is not implied. A more accurate appelation might be unsaturated ferromagnetism. Still more accurately, ferrimagnetism might be the right word—but technically that word implies a spatial ordering that I am not prepared to prove. In one dimension $|B|=|A|$ by definition and therefore $S=0$; this conclusion coincides with the known result[8] that S is always zero in one dimension with nearest-neighbor nonpositive hopping $t_{xy}\leq 0$ and for *any many-body potential.* There is also the example of Thouless and Nagaoka[9–11] with $N=|\Lambda|-1$, $U=\infty$, and $2S=|\Lambda|-1$, but infinite potentials are crucial for this example.

(6) Theorem 2 also has some extensions similar to some of those described in remark (2) above; hole-particle symmetry is required.

Proof of theorem 1.—S^2 and S^z are conserved and I work in the $S^z=0$ subspace since all competitors have a representative there. That is to say, each eigenstate with a given S value can (by the well known properties of angular momentum) be rotated in spin space to a state with $S_z=0$ without changing its energy. Then there are $n=\frac{1}{2}N$ electrons of each type, spin up and spin down. Let $\{\psi^{\alpha}\}$ be any orthonormal basis for *one species* of n spinless fermions; there are

$$m=\binom{|\Lambda|}{n}$$

of these and I require that they be *real* (i.e., each ψ^{α} is a *real,* homogeneous polynomial of order n in the $c_x^{\dagger}$'s acting on the vacuum). A ground state ψ can then be written as $\psi=\sum_{\alpha,\beta}W_{\alpha\beta}\psi_{\uparrow}^{\alpha}\otimes\psi_{\downarrow}^{\beta}$ with $W_{\alpha\beta}$ as coefficients. This $W_{\alpha\beta}$ is here viewed as a $m\times m$ matrix. Because all operators and basis vectors are real and because the Hamiltonian is symmetric between the up and the down spins, it is obvious that if $W_{\alpha\beta}$ corresponds to a ground state then so does $W_{\beta\alpha}^{*}=(W^{\dagger})_{\alpha\beta}$, and hence (by linearity) so does $W+W^{\dagger}$ and $i(W-W^{\dagger})$. Thus, for conveni-

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ence, we may henceforth assume $W=W^{\dagger}$ (but $W_{\alpha\beta}$ is not assumed to be real). The norm of ψ squared is $\langle\psi|\psi\rangle=\sum_{\alpha,\beta}|W_{\alpha\beta}|^2=\mathrm{Tr}W^2$ and I assume that this is unity. The hopping energy part of $\langle\psi|H|\psi\rangle$ is easily found to be $2\,\mathrm{Tr}KW^2$ where

$$K_{\alpha\beta}=\langle\psi^{\beta}|\sum_{x,y}t_{xy}c_x^{\dagger}c_y|\psi^{\alpha}\rangle\,.$$

Clearly K is real and symmetric since each t_{xy} is real. The on-site energy is given by $-\sum_x U_x\,\mathrm{Tr}(WL_xWL_x)$ with $(L_x)_{\alpha\beta}=\langle\psi^{\beta}|n_x|\psi^{\alpha}\rangle$, which is also real and symmetric. The total energy is then

$$E(W)=\langle\psi|H|\psi\rangle=2\,\mathrm{Tr}KW^2+\sum_x U_x\,\mathrm{Tr}(WL_xWL_x)\,, \quad (3)$$

and the equation for W, corresponding to the eigenvalue equation $H\psi=e\psi$, is

$$KW+WK+\sum_x U_xL_xWL_x=eW\,. \quad (4)$$

Now consider the positive semidefinite matrix $|W|$ defined by $|W|^2=W^2$. Obviously, $\mathrm{Tr}W^2=\mathrm{Tr}|W|^2$. Moreover, in an orthonormal basis (not to be confused with the ψ^{α} basis for the electrons) in which the Hermitian $m\times m$ matrix W is diagonal, with diagonal elements w_i, the Hermitian matrix $|W|$ is also diagonal with elements $|w_i|$. In this diagonal basis I compute

$$\mathrm{Tr}WL_xWL_x=\sum_{i,j}w_iw_j|(L_x)_{ij}|^2\le\sum_{i,j}|w_i||w_j||(L_x)_{ij}|^2$$
$$=\mathrm{Tr}|W|L_x|W|L_x\,.$$

Since $U_x\le 0$, I conclude that $E(W)\ge E(|W|)$ and therefore that *among the ground states there is one satisfying* $W=|W|\ge 0$. This is the "spin-space reflection positivity" mentioned in the second paragraph. (This part of the proof is an adaptation of that given in Ref. 4.) I choose this positive (possibly semidefinite) matrix W and now make the choice that the ψ^{α}'s are the natural x-space basis for the electrons, i.e., α denotes n points in Λ and $\psi^{\alpha}=\prod_{x\in\alpha}c_x^{\dagger}|0\rangle$. (Some arbitrary convention for the sign of the ψ^{α}'s can be made here.) Since $W\ge 0$, it follows that $W_{\alpha\alpha}>0$ for at least one α, for otherwise W vanishes identically. However, the vector $\phi^{\alpha}=\psi_{\uparrow}^{\alpha}\otimes\psi_{\downarrow}^{\alpha}$ satisfies $(S_{\mathrm{op}})^2\phi^{\alpha}=0$ and therefore this ground state ψ has a nonzero projection onto the eigenspace of $(S_{\mathrm{op}})^2$ in which $S=0$. This would be impossible if conclusion (a) were false and thus conclusion (a) must be true.

To prove conclusion (b) I shall prove that necessarily a Hermitian W satisfies $W=|W|$ or $W=-|W|$ for every ground state when $U_x<0$ for every x. This will prove conclusion (b) for the following reason. If there were two normalized, Hermitian ground state W's, say W^1 and W^2 with $W^1\neq\pm W^2$, then for every real constant d, the Hermitian matrix $W^1+dW^2\equiv W_d$ is not zero and defines (after normalization) a ground state, by virtue of the linearity of the eigenvalue Eq. (4). It is easy to verify that there must be a d for which W_d is neither positive nor negative semidefinite, and this contradicts the assertion that the ground state W_d satisfies $W_d=\pm|W_d|$.

With W given then, consider the Hermitian, positive semidefinite matrix $R\equiv|W|-W$ which is also a multiple of a ground state and satisfies (4). If Q denotes the kernel of R, i.e., $Q=\{\text{vectors } V \text{ such that } RV=0\}$, then the assertion $W=\pm|W|$ is implied by the following statement which I shall prove: Q is either just the zero vector or else every vector is in Q. Let V be in Q and take the expectation of (4) in this state V, i.e.,

$$\langle V|KR+RK+\sum_x U_xL_xRL_x|V\rangle=e\langle V|R|V\rangle\,.$$

Since $RV=0$ and, for all x, $U_x<0$ and $\langle V|L_xRL_x|V\rangle\ge 0$ by the positive semidefiniteness of R, I conclude that $\langle V|L_xRL_x|V\rangle=0$ for all x. Since R is positive semidefinite, I conclude that $RL_xV=0$. Thus each L_x maps Q into Q. Now let the matrices in (4) act on V (without taking expectation values). Since $RL_xV=0$ and $RV=0$, I conclude that $RKV=0$. Thus K also maps Q into Q. As before, let α denote a collection of n points in Λ and define $L^{\alpha}=\prod_{x\in\alpha}L_x$, which is the projector onto the basis vector μ^{α} in C^m [with components $(\mu^{\alpha})_{\gamma}=\delta_{\alpha\gamma}$] and which has matrix elements $(L^{\alpha})_{\gamma\delta}=\delta_{\alpha\gamma}\delta_{\gamma\delta}$. Note that the L_x's commute with each other and so the ordering of the L_x's is unimportant in the definition of L^{α}. Each L^{α} maps Q into Q because each L_x does. Since Λ is connected by T, it is easy to see that the α's are connected by K, i.e., for all α and β there are indices $\gamma_1,\gamma_2,\ldots,\gamma_p$ for some integer p such that the ordinary (not matrix) product $G_{\beta\alpha}\equiv K_{\beta\gamma_1}K_{\gamma_1\gamma_2}\cdots K_{\gamma_p\alpha}$ is not zero. If Q is not just the zero vector and $V\neq 0$ is in Q then $L^{\alpha}V\neq 0$ for some fixed choice of α (because $\sum_{\alpha}L^{\alpha}$ is the identity). Then $L^{\alpha}V=z\mu^{\alpha}$ for some nonzero constant z and with μ^{α} being the aforementioned basis vector. But then the vector $F\equiv L^{\beta}KL^{\gamma_1}K\cdots L^{\gamma_p}KL^{\alpha}V$ is in Q and, in fact, $F=zG_{\beta\alpha}\mu^{\beta}$. In short, Q contains a complete set of vectors (i.e., every μ^{β}) because $G_{\beta\alpha}$ is nonzero for every β by virtue of the connectivity. Thus every vector is in Q since Q is a linear space, which implies that $W=\pm|W|$ and which, in turn, implies uniqueness of the ground state. Q.E.D.

Proof of theorem 2.—First make the conventional unitary hole-particle transformation for the spin-up electrons followed by a sign change on the B sublattice, i.e., $c_{x\uparrow}\to\epsilon(x)c_{x\uparrow}^{\dagger}$ and $c_{x\uparrow}^{\dagger}\to\epsilon(x)c_{x\uparrow}$ with $\epsilon(x)=1$ for $x\in A$, $\epsilon(x)=-1$ for $x\in B$. The spin-down electrons are unaltered, i.e., $c_{x\downarrow}\to c_{x\downarrow}$. Then $n_{x\uparrow}\to 1-n_{x\uparrow}$ and the transformed H is $\tilde{H}+UN_{\downarrow}$ with

$$\tilde{H}=\sum_{\sigma}\sum_{x,y\in\Lambda}t_{xy}c_{x\sigma}^{\dagger}c_{y\sigma}-U\sum_{x\in\Lambda}n_{x\uparrow}n_{x\downarrow}\,, \quad (5)$$

and with $N_{\sigma}=\sum_x n_{x\sigma}$. The original number operators N_{σ} transform as $N_{\downarrow}\to\tilde{N}_{\downarrow}=N_{\downarrow}$ and $N_{\uparrow}\to\tilde{N}_{\uparrow}=|\Lambda|-N_{\uparrow}$. The original condition $N=|\Lambda|$ becomes $N_{\uparrow}=N_{\downarrow}$. The

spin operators (2) become the *pseudo-spin operators*

$$\tilde{S}^z = \tfrac{1}{2}(|\Lambda| - N_\uparrow - N_\downarrow), \quad \tilde{S}^+ = \sum_{x \in \Lambda} \epsilon(x) c_{x\uparrow} c_{x\downarrow}, \qquad (6)$$

and $S^2 \to (\tilde{S}^z)^2 + \frac{1}{2}\tilde{S}^+\tilde{S}^- + \frac{1}{2}\tilde{S}^+\tilde{S}^+ \equiv (\tilde{S})^2$. The $\tilde{S}$ operators commute with $\tilde{H}$, but so do the spin operators S given in (2). The S operators are the transforms of the pseudo-spin operators in the original variables and are of no special physical interest. The $\tilde{S}$ operators are the ones of interest as far as $\tilde{H}$ is concerned.

As before, I can work in the $\tilde{N}_\uparrow = \tilde{N}_\downarrow = |\Lambda|/2$ subspace, which implies that $N_\uparrow = N_\downarrow = |\Lambda|/2$. The uniqueness part of theorem 2 is then a consequence of conclusion (b) of theorem 1, which also states that the unique ground state $\tilde{\psi}$ of $\tilde{H}$ has $S = 0$. This last fact is of secondary importance. The real problem is to prove that $2\tilde{S} = |B| - |A|$. The shortest proof is to return to H and the $S^z = 0$ subspace (in the *original variables).* For each $U > 0$ the ground state $\psi(U)$ is nondegenerate as has been shown and I want to prove that $2S = |B| - |A|$. The nondegeneracy of the ground state for *all* $U > 0$ implies that the S of this unique ground state must be independent of U, for otherwise continuity in U would imply a degeneracy for some value of $U > 0$. However, when U is very large, H, as stated before, is equivalent (to leading order in U) to h, the Heisenberg antiferromagnetic Hamiltonian defined in remark (4). As stated there, h *also* has a unique ground state[6] (for $S^z = 0$) and this state has $2S = |B| - |A|$. The uniqueness property of h is crucial for it implies a gap (however small it may be) in the spectrum of h. Thus, for large enough U the S value of the ground state of h is identical to that of H. Q.E.D.

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THE HUBBARD MODEL: SOME RIGOROUS RESULTS AND OPEN PROBLEMS

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ABSTRACT

The Hubbard model of interacting electrons, like the Ising model of spin-spin interactions, is the simplest possible model displaying many "real world" features, but it is much more difficult to analyze qualitatively than the Ising model. After a third of a century of research, we are still not sure about many of its basic properties. This mini-review will explore what is known rigorously about the model and it will attempt to describe some open problems that are possibly within the range of rigorous mathematical analysis.

0. INTRODUCTION

The Hubbard model is to the problem of electron correlations as the Ising model is to the problem of spin-spin interactions; it is the simplest possible model displaying many "real world" features. It is, however, much more difficult to analyze qualitatively than the Ising model. After a third of a century of research, we are still not sure about many of its basic features. It is believed, for example, to have something to do with high temperature superconductivity, and it would be nice to validate this.

One of the most intriguing questions concerns magnetism — particularly the magnetic properties of the ground state. The familiar models of interacting spins, such as the Ising or Heisenberg models, posit an underlying spin Hamiltonian that ultimately comes from a model of itinerant electrons. The mystery here is that neither

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the electronic kinetic nor the electronic potential energies favor ferromagnetism, but together they sometimes do so. Ferromagnetic spin models, for example, are popular, but the truth is that the antiferromagnetic preference of the kinetic energy usually seems to dominate. In fact the only known examples of saturated itinerant electron ferromagnetism come from the Hubbard model in a special limit (infinite repulsion and one hole) devised by Nagaoka [NY] or from the Hubbard model with finite repulsion but on special lattices devised by Mielke and Tasaki [Mi1, TH2, MT] for which the kinetic energy spectrum is macroscopically degenerate. No doubt, further study of the Hubbard model will eventually lead to a better understanding of the way in which the Pauli exclusion principle leads to magnetism.

These notes will explore what is known rigorously about the model and they will attempt to describe some open problems that are possibly within the range of rigorous mathematical analysis. The notes are not a complete review in the sense that every contribution is covered, but an attempt has been made to mention, at least, most topics that can be treated rigorously. I apologize to those authors whose works have been omitted and I hope this will be attributed to my ignorance rather than intent. Given more space I would have liked to discuss the closely related Falicov-Kimball model, for which many rigorous results are known, but which is not a Hubbard model because it does not have $SU(2)$ symmetry. Another interesting chapter would be the infinite dimensional Hubbard model—pioneered by Metzner and Vollhardt [MV]—and which opens exciting mathematical and physical avenues. It has led to a large literature, but much remains to be added in the way of mathematical rigor.

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I. DEFINITION OF THE MODEL

Only the original short-range Hubbard model will be considered here. Like the Ising model, the Hubbard model is defined on a graph, i.e., a collection of vertices or sites (denoted by Λ and whose number is $|\Lambda|$) and (unordered) edges or bonds connecting certain distinct pairs of vertices. The word graph instead of lattice is used to avoid any possible implication of translation invariance because most of the results stated here do not depend on such invariance. One is given a **hopping matrix** T, with elements t_{xy}, with x and $y \in \Lambda$, and we assume, as a convention, that $t_{xy} = 0$ if x, y are not connected by an edge. Note that $t_{xx} = 0$. t_{xy} might be complex, signaling the presence of a magnetic field, the line integral of whose vector potential from x to y (thought of now as points in $\mathbf{R}^3$) is $\arg(t_{xy})$. However, T is always self adjoint, $t_{xy} = t^*_{yx}$, with $*$ denoting complex conjugate.

The **bipartite** graphs form an important sub-class; here $\Lambda = A \cup B$, with A and B disjoint, and such that there is no edge between x, y if $x \in A$ and $y \in A$ or if $x \in B$ and $y \in B$. The square lattice is bipartite, the triangular is not.

Electrons, i.e., spin $\frac{1}{2}$ fermions, move on Λ with kinetic energy given in second quantized form by $K = K_\uparrow + K_\downarrow$ with

$$K_\sigma = -\sum_{x,y\in\Lambda} t_{xy} c^\dagger_{x\sigma} c_{y\sigma}. \tag{1.1}$$

Here $\sigma = \pm 1$ denote the two spin states $\uparrow$ and $\downarrow$ while $c^\dagger_{x\sigma}$ is the creation operator for an electron at x with spin σ. We have $c^\dagger_{x\sigma}c_{y\tau} + c_{y\tau}c^\dagger_{x\sigma} = \delta_{xy}\delta_{\sigma\tau}$ and $c_{x\sigma}c_{y\tau} + c_{y\tau}c_{x\sigma} = 0$. The number operator is defined by $n_{x\sigma} = c^\dagger_{x\sigma}c_{x\sigma}$ and has eigenvalues 0 and 1. The total number of each spin species

$$N_\sigma = \sum_{x\in\Lambda} n_{x\sigma}$$

is a conserved quantity. The total particle number is $N = N_\uparrow + N_\downarrow$ which satisfies $0 \le N \le 2|\Lambda|$. The **half-filled band**, $N = |\Lambda|$ is especially important and especially amenable to analysis.

In the physics literature it is often assumed that $t_{xy} =$ constant $= t > 0$ on all edges of Λ, in which case T is a discrete version of the Laplacian, but without the diagonal terms. This assumption will not generally be made here.

At each site x there is also given a number U_x which governs the on-site electron-electron interaction at x. We usually assume all $U_x \ge 0$ (repulsive case) or all $U_x \le 0$ (attractive case). The total potential energy is[†]

$$W = \sum_{x\in\Lambda} U_x(n_{x\uparrow} - \tfrac{1}{2})(n_{x\downarrow} - \tfrac{1}{2}). \tag{1.2}$$

The total Hubbard Hamiltonian of our system is then

$$H = K + W, \tag{1.3}$$

and most of the results discussed here are about the ground state of this H. In fact, many of the results do not require a point interaction as in (1.2); instead, terms like $U_{xy}(n_{x\uparrow} - \frac{1}{2})(n_{y\downarrow} - \frac{1}{2})$, with the matrix U_{xy} being positive semidefinite, are also allowed.

The interaction in (1.2) includes a one-body term $-\frac{1}{2}\sum_x U_x(n_{x\uparrow} + n_{x\downarrow})$ plus a trivial constant term $\frac{1}{4}\sum_x U_x$. If U_x is independent of x, as is normally assumed in almost all papers on the subject, then this one-body term is trivially a constant proportional to the fixed particle number. It is interesting to consider $U_x \neq$ constant, and the one-body term is included in (1.2) in order to be able to exploit **hole-particle symmetry**: The unitary transformation that maps $c_{x\downarrow} \to c^\dagger_{x\downarrow}$ and $c^\dagger_{x\downarrow} \to c_{x\downarrow}$ (but $c_{x\uparrow} \to c_{x\uparrow}$) is the hole-particle transformation on the down-spins and it maps $(n_{x\downarrow} - \frac{1}{2})$ into $-(n_{x\downarrow} - \frac{1}{2})$. Thus, this transformation maps the repulsive W into the attractive W and vice versa, but it changes the down-spin number from $N_\downarrow$ to $|\Lambda| - N_\downarrow$.

This hole-particle transformation may or may not map $K_\downarrow$ into $K_\downarrow$. It does map $K_\downarrow$ into $\widehat{K}_\downarrow$, defined by $\widehat{t}_{xy} = -t^*_{yx}$.

In the special, but important case that T is real and Λ is bipartite we can make a further unitary transformation that will take $\widehat{K}_\downarrow$ into $K_\downarrow$ and $n_{x\downarrow}$ into $n_{x\downarrow}$. This unitary transformation maps $c_{x\downarrow}$ into $(-1)^x c_{x\downarrow}$ (and, of course, $c_{x\uparrow}$ into $c_{x\uparrow}$), where

[†] The usual formulation is $n_\uparrow n_\downarrow$ instead of our $(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$. If U_x varies with x the two formulations are obviously inequivalent. The formulation here is not without a physical foundation because a neutral atom (with $n_\uparrow + n_\downarrow = 1$) is locally the most stable configuration and adding or removing an electron produces a net local charge that raises the energy roughly equally.

$(-1)^x$ denotes the function on the vertices of Λ which is $+1$ for $x \in A$ and -1 for $x \in B$. Effectively, t_{xy} is mapped into $(-1)^x(-1)^y t_{xy} = -t_{xy}$ for the down-spins. Henceforth, the hole-particle transformation on bipartite lattice is always meant to include this additional unitary $(-1)^x$, so that $K_\downarrow$ is mapped into $K_\downarrow$.

Thus, in the special real, bipartite case we can analyze the repulsive case by analyzing the attractive case. But we have to remember that $N_\downarrow \leftrightarrow |\Lambda| - N_\downarrow$ so that the particle number for one is related to the magnetization of the other. This is a non-trivial distinction and is similar to the relation between the ferromagnetic and antiferromagnetic Ising models on a bipartite graph.

The hole-particle transformation also induces a conservation law in the real, bipartite case that has no classical analogue. Like any electron system this model has an $SU(2)$, i.e., angular momentum, invariance. The generators are

$$J^3 = \tfrac{1}{2}(N_\uparrow - N_\downarrow), \qquad J^+ = \sum_{x\in\Lambda} c^\dagger_{x\uparrow} c_{x\downarrow}, \qquad J^- = (J^+)^\dagger. \tag{1.4}$$

However, the Hamiltonian H in (1.3) is the unitary transform (described above) of another H' (with U_x replaced by $-U_x$) which also has an $SU(2)$ symmetry with generators given by (1.4) in the *transformed* basis. By transforming back we obtain a different set of $SU(2)$ generators

$$\widehat{J}^3 = \tfrac{1}{2}(N_\uparrow + N_\downarrow - |\Lambda|), \qquad \widehat{J}^+ = \sum_{x\in\Lambda} (-1)^x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow}, \qquad \widehat{J}^- = (\widehat{J}^+)^\dagger \tag{1.5}$$

that also commute with H and with the J's in (1.4). We call this the **pseudospin**. This special model thus has an $SU(2)\times SU(2)$ symmetry group,[§] but it must be emphasized that real T is *essential* (zero magnetic field). These operators change the quantum numbers $N_\uparrow$ and $N_\downarrow$. The operators $J^\pm$ change J^3 by one unit while $\widehat{J}^\pm$ change $\widehat{J}^3$ by one unit. The four operators together thus permit us to move around inside rectangles in $(N_\uparrow, N_\downarrow)$ space whose four vertices have the form $(n,m), (m,n), (|\Lambda|-n, |\Lambda|-m), (|\Lambda|-m, |\Lambda|-n)$. This means that to each eigenstate for $N_\uparrow = n$, $N_\downarrow = m$ there is a corresponding eigenstate with the same energy at each point (n', m') in the rectangle with $n' + m' = n + m \pmod 2$ (there are also additional eigenstates, of course). Thus, the usual operators $J^\pm$ permit us to infer all the states of our Hamiltonian from knowledge of the states on the line $N_\uparrow - N_\downarrow = 0$ or the line $N_\uparrow - N_\downarrow = 1$. The pseudospin operators $\widehat{J}^\pm$ permit us to infer everything from knowledge of the line $N_\uparrow + N_\downarrow = |\Lambda|$ (half-filled band) or the line $N_\uparrow + N_\downarrow = |\Lambda| + 1$. But we repeat that this property of $\widehat{J}^\pm$ holds *only* for the real, bipartite case.

We note, for future use, that the hole-particle transformation (*without* $(-1)^x$) applied to *both* spins (namely $c_{x\sigma} \leftrightarrow c^\dagger_{x\sigma}$). does not preserve $\vec{J}$. Indeed, $J^3 \to -J^3$, $J^\pm \to -J^\mp$, but $\mathbf{J}^2 \to \mathbf{J}^2$.

The Hubbard model describes — in the simplest possible fashion — an interacting fermion system. It can be viewed this way, as a toy model, or it can be viewed,

[§] Actually, the group is $SO(4) = SU(2) \times SU(2)/Z_2$, as pointed out by Yang and Zhang [YZ]. The reason is that the two operators $w = -\mathbf{1}$ in each $SU(2)$ corresponds to only *one* operator on our Hilbert space, i.e., $w \otimes \mathbf{1} = \mathbf{1} \otimes w$. This reduction to $SO(4)$ coincides with the observation that in every state the spin and pseudospin are either both integral or both half-integral when $|\Lambda|$ is even.

a bit more realistically in the repulsive case, as a serious model of π-electrons hopping between localized Wannier orbitals in some molecule such as benzene (with $|\Lambda| = 6$); the half-filled band, $N = |\Lambda|$, is then especially important because it corresponds to neutrality. The ultra-short range interaction is supposed to mimic a highly screened Coulomb potential. From the latter viewpoint it was known first in the chemistry literature as the Pariser-Parr [PP]-Pople [PJ] model; molecules having a bipartite structure are called "alternant molecules". It was a decade later that Hubbard [HJ], Gutzwiller [GMC] and Kanamori [KJ] realized its importance for bulk matter.

II. ONE-DIMENSIONAL EXACTLY SOLVABLE MODEL

In 1968 the ground state of H was solved for the translation invariant one-dimensional ring by Lieb and Wu [LW] using the extension of the "Bethe ansatz" technique [BH, LL1] to fermions [MJ, FL1, YC, GM]. Shortly thereafter, Ovchinnikov [OA] used these results to calculate the elementary excitation spectrum at half filling. Recently, Essler and Korepin [ES] obtained a new and illuminating derivation. Coll [CC] extended Ovchinnikov's results to arbitrary filling, as did Woynarovich [WF]. Takahashi [TM] evaluated the magnetism curve at half filling and Shiba [SH] evaluated the magnetic susceptibility for all filling. Koma [KO] has formulated a sequence of approximations to the positive temperature free energy and correlation length (obtained by using the Trotter product formula for the partition function) which converge to the exact answer and such that each approximation can be calculated using the Bethe ansatz without any assumptions, such as the "string hypothesis".

These results were obtained in the thermodynamic limit, in which sums could be replaced by integrals. Woynarovich and Eckle [WE] evaluated the asymptotics of finite size effects on the ground state energy. For small chains the general "Bethe ansatz" solution, while correct, is too complicated for numerical evaluation. Heilmann and Lieb [HL] undertook to evaluate *all* the energy levels for *all* $U > 0$ for the benzene molecule ($N = 6, |\Lambda| = 6$). To our surprise we found many instances of both level crossings and of permanent degeneracy — as a function of U — and which were not accounted for on the basis of the known invariance groups (spin, pseudospin and symmetries of the hexagon). This means that the system has *non-abelian* symmetry groups and these *are dependent on* U (i.e., the group operations commute with H but *not* with K and W separately; a well known example of this phenomenon, for the hydrogen atom, is the Runge-Lenz vector whose definition depends on the value of the electron's charge).

What are these invariants? Sixteen years later Shastry [SB] (unaware of [HL]) found many invariants and also a two-dimensional classical statistical mechanics vertex model whose transfer matrix commutes with our H. In fact he found a whole commuting family of such transfer matrices — which means that the one-dimensional model can be called "integrable". In view of the non-abelian symmetries mentioned above for the six-site model, it is not clear whether all invariants of H are, in general, of Shastry's form. A few years later, Grosse [GH] (motivated by [HL]) published another derivation of some of the invariants.

Another interesting question is whether all the eigenstates of H are of the "Bethe ansatz" form. This was answered in the negative by Essler, Korepin and Schoutens [EKS] who went on to demonstrate that when the ring is bipartite (i.e., even length)

the $SU(2) \times SU(2)$ generators J^+ and $\widehat{J}^+$ save the day. The lowest weight states (the ones that are annihilated by J^- and $\widehat{J}^-$) are claimed to be *all* of the "Bethe ansatz" type. All the remaining states are then obtained by application of J^+, and $\widehat{J}^+$.

Many of the "Bethe Ansatz" results rely on a "string" hypothesis. Moreover, some assertions in [EKS], notably the linear independence of the solutions, rely on an appeal to some properties of Shastry's invariants that have not been verified. It is desirable to put these matters on a more rigorous basis.

The literature about this one-dimensional solution is vast and the above remarks do not reflect everything that is known about the subject.

III. MAGNETISM

A. One-Dimension

It is convenient, now, to take an open chain instead of a ring. Then, by a general theorem of Lieb and Mattis [LM1], whose proof also works for lattice systems with nearest neighbors hopping and a *completely arbitrary* many-body potential, $E^N(S)$, the ground state energy of H, as a function of total spin $S \leq \frac{1}{2}N$ and for N particles, satisfies

$$E^N(\tfrac{1}{2}N) > E^N(\tfrac{1}{2}N - 1) > E^N(\tfrac{1}{2}N - 2) > \ldots > E^N(0) \text{ or } E^N(\tfrac{1}{2}). \qquad (3.1)$$

The numbers U_x are now totally arbitrary and not necessarily of one sign. [Note: The original theorem [LM1] uses a Perron-Frobenius positivity argument, which a-priori requires $t_{xy} > 0$. However, any T can be reduced to this form in one-dimension by the simple unitary gauge transformation $c_{x\sigma} \to \exp[-i\theta(x)]c_{x\sigma}$, which carries t_{xy} into $\widehat{t}_{xy} := t_{xy} \exp[i\theta(x) - i\theta(y)]$, where $\theta(x)$ is an arbitrary real number, selected so that $\widehat{t}_{xy} > 0$ for all x and y.] Since we can then take T to be real, our H is then the (down-spin) hole-particle transform of some other $\widehat{H}$, in which U_x is replaced by $-U_x$. Assuming N to be even, (3.1) says that the ground state of H has $N_\uparrow = N_\downarrow = N/2$. The transformed $\widehat{H}$ system has $\widehat{N}_\uparrow = N_\uparrow$, $\widehat{N}_\downarrow = |\Lambda| - N_\downarrow$, whence $\widehat{S}^3 = \frac{1}{2}(\widehat{N}_\uparrow - \widehat{N}_\downarrow)$ is the predetermined number $\frac{1}{2}(N - |\Lambda|)$. The $\widehat{H}$ system also satisfies (3.1) since it is one-dimensional, and the spin of the ground state of the $\widehat{H}$ system is therefore

$$\widehat{S} = \tfrac{1}{2}\big|N - |\Lambda|\big|.$$

This number, $\widehat{S}$, is *the pseudospin of our ground state* — a curious result whose physical significance is not entirely obvious. (Note the logic here. Both systems, H and $\widehat{H}$ must be in their respective ground states, consistent with the given conditions on each; for H it is $N_\uparrow + N_\downarrow = N$ and for $\widehat{H}$ it is $N_\uparrow - N_\downarrow = N - |\Lambda|$.)

This theorem was extended many years later by Aizenman and Lieb [AL] to positive temperatures. The main theorem, applicable to any many-body potential in a one-dimensional system, expresses the fact that the free energy is a monotone increasing function of the spin. This is done in terms of total spin S or 3-component s, as follows; neither inequality implies the other.

Classify the eigenstates by the 3-component of spin, $J^3 = s = \frac{1}{2}(N_\uparrow - N_\downarrow)$, and by S, the total spin angular momentum (recall $\mathbf{J}^2 = S(S+1)$). For a given N and

inverse temperature β, let $Z_3(s) = \mathrm{Tr}_s e^{-\beta H}$ be the partition function in which only states of a given s value are included. Likewise, let $Z_J(S) = \mathrm{Tr}_S e^{-\beta H}$ be the partition function for a given S. We have the relation $Z_3(S) - Z_3(S+1) = (2S+1)^{-1} Z_J(S)$, which is obvious from the theory of angular momentum. Correspondingly, we have the combinatorial quantities $Y_3(s) := \binom{N}{\frac{N}{2}+s}$ and $Y_J(S) := (2S+1)[Y_3(S) - Y_3(S+1)]$, which are essentially the partition functions of free particles with $H = 0$, and which serve to normalize the Z's. The two theorems are then that

$$\frac{Z_3(s)}{Y_3(s)} \quad \textit{and} \quad \frac{Z_J(S)}{Y_J(S)}$$

are *both strictly monotone decreasing functions of their arguments* (s or S). A corollary of this is that the magnetization is less than its value in the **atomic limit** (or what I prefer to call the pure paramagnetic value). I.e., for all β and magnetic field h

$$M(\beta, h) = \frac{1}{\beta} \frac{\mathrm{d}}{\mathrm{d}h} \ln Z(h) < N \tanh(\beta h). \tag{3.2}$$

Here $Z(h) = \sum_{s=-N/2}^{N/2} Z_3(s) \exp[2\beta s h]$ is the total partition function (recall that the g-factor of an electron is 2).

It is noteworthy that all this holds for *completely arbitrary*, Hermitian t_{xy} and (real) U_x. Indeed, it holds even if we add an arbitrary real one body potential

$$V = \sum_{x \in \Lambda} V_x (n_{x\uparrow} + n_{x\downarrow}).$$

An amusing fact about one-dimension concerns the $U = +\infty$ case. For an open chain the ground state is highly degenerate—indeed, it can have any value of S. For a closed chain the situation is quite different and the S of the ground state depends on the sign of the t_{xy}'s and whether N is even or odd; S can be $N/2$ in some cases [AL]. The situation is discussed in detail by Mielke [Mi2] who finds that the "average" S is $\sqrt{N}$. Some interesting facts about the closed one-dimensional chain with $U = 0$, but with a magnetic field, can be found in [LL2]. The $U \neq 0$ case is discussed by Fujimoto and Kawakami [FK1].

B. Half-Filled Band

The hole-particle symmetry notwithstanding, the repulsive case (all $U_x \geq 0$) and the attractive case (all $U_x \leq 0$) are quite different, even for a bipartite lattice. The physical spin of one is the pseudospin of the other.

In the limit $U \to +\infty$ (by which I mean all $U_x \to +\infty$), the energy and wave functions have nice limits. The electrons become hard-core particles. When $N = |\Lambda|$ we just have one electron per site and, since motion is impossible, each electron can be, independently, spin-up or spin-down. This gives us the atomic limit whose partition function is Y_3 or Y_J given above. First order perturbation theory in t/U vanishes, but in second order we have to diagonalize our H among all the $2^{|\Lambda|}$ degenerate ground states just described. This yields an effective Hamiltonian H' that can be written in terms of the three Pauli spin operators $\mathbf{S}$ at each site. It turns out [AP] that for any graph

$$H' = \sum_{x,y \in \Lambda} J_{xy}(\mathbf{S}_x \cdot \mathbf{S}_y - \tfrac{1}{4}) \tag{3.3}$$

with $J_{xy} = |t_{xy}|^2(U_x^{-1} + U_y^{-1})$. This is the spin 1/2 antiferromagnetic Heisenberg Hamiltonian and it is known [LE1, LM2] that its ground state has total spin

$$S = \big||A| - |B|\big| \tag{3.4}$$

on a bipartite graph. It is also known [DLS, KLS] that in the **translation invariant case** (i.e., our graph is a D-dimensional hypercube with periodic boundary conditions and $t_{xy} = \text{constant} = t$ and $U_{xy} = \text{constant} = U$) there is long range order when $D \geq 3$.

The obvious question is whether the results just stated (i.e., (3.4) and the long range order) hold non-perturbatively in the repulsive case. One would also guess that in the attractive case the total spin should be zero in the ground state because when $U_x = -\infty$ for all x the ground state consists simply of bound pairs of electrons sitting on selected sites. These questions about the spin are answered in the following [LE1].

Theorem 1: *Assume t_{xy} is real for all $x, y \in \Lambda$. If $U_x < 0$ for all x, the ground state on any connected graph is unique and has spin $S = 0$* for any even electron number, N, not just $N = |\Lambda|$. *If $U_x > 0$ for all x, if Λ is connected and bipartite and if $N = |\Lambda|$ is even, the ground state is unique (except for the $(2S+1)$-fold degeneracy) and has spin $S = \frac{1}{2}\big||A| - |B|\big|$.*

We can easily have $|A| - |B|$ of the order of $|\Lambda|$ itself. As an example, take a square lattice and add a site at the center of each bond of this square lattice. The original sites are then B sites and the new sites are A sites. Then $|A| = 2|B|$ and the ground state has a bulk magnetization per site of 1/3. This is really more like ferrimagnetism than ferromagnetism but, in any case, it is one of the few examples known in which the system has a bulk magnetization without an external magnetic field. Note that a one-dimensional chain always has $\big||A| - |B|\big|$ equal to 0 or 1, and thus Theorem 1 coincides with (3.1) in this case.

There is an interesting corollary of this theorem if Λ is bipartite, $|\Lambda|$ is even and $|A| > |B|$. Suppose we ask for the absolute minimum energy, without fixing N. Starting with $U_x > 0$ we find that an optimum N is $N = |\Lambda|$ or $|\Lambda| + 1$ (by the $SU(2) \times SU(2)$ symmetry mentioned in Sec. 1); by repeating the proof of Theorem 1, one can show $N = |\Lambda|$. But $J^3 = (N_\uparrow - N_\downarrow)/2$ can be any integer in the interval

$(|B| - |A|)/2$ to $(|A| - |B|)/2$ since $S = (|A| - |B|)/2$. Now using hole-particle symmetry to obtain the $U_x < 0$ model, we find that the optimum N is any even integer satisfying $2|B| \leq N \leq 2|A|$. (E.g., starting with $N_\uparrow = |A|, N_\downarrow = |B|$, the transformed values are $N_\uparrow = |A|, N_\downarrow = |\Lambda| - |B|$, which yields $N = 2|A|$.) Thus, *there can be a large degeneracy in the attractive case!* (For $U = 0$ this is easily seen from the remark that T has at least $|A| - |B|$ zero eigenvalues.)

Theorem 1 is based on a certain "positive definite" property of the ground state, proved in [LE1]. This property was used by Tian [TG4] to prove some interesting facts about off-diagonal long range order. Shen and Qiu [SQ] also used this positive definiteness to prove that the negative U Hubbard model on a bipartite lattice has off-diagonal long-range order for a certain range of electron densities when $|A| \neq |B|$. Motivated by [TG4], Shen, Qiu and Tian [SQT2] used the same hypotheses and method to show ferrimagnetic long-range order in the positive U model at half-filling. This is the first example of its kind for an itinerant electron model. The obvious open problem is to remove the restriction $|A| \neq |B|$, but the results in [LE1] do not seem to shed light on this. In particular, the long-range order in [SQT2] holds even in one-dimension, but when $|A| = |B|$ we do *not* expect to find long-range order in one-dimension, even in the ground state. (Note: We can make a "one-dimensional" model with $|A| = 2|B|$ by taking the usual one-dimensional chain and adding an A-site at the side of every B-site.)

Theorem 1 was extended to positive temperature by Kubo and Kishi [KK] who found upper bounds on certain two-point functions. They discuss only the translation invariant case on a hypercubic lattice with $U_x = U =$ constant, but their method easily extends to the general case. For $U < 0$ they bound the spin susceptibility at wave vector q by

$$\chi_q \leq \frac{1}{4|U|} \tag{3.5}$$

for all temperatures and all filling fraction $N/|\Lambda|$ (more precisely, they use the grand canonical ensemble and prove (3.5) for all chemical potentials μ). This result precludes magnetic long range order. In the repulsive case $U > 0$, and with μ adjusted to the half-filled band case $N = |\Lambda|$, namely $\mu = 0$, they bound the charge susceptibility as

$$(\delta\widehat{n}_q, \delta\widehat{n}_{-q}) \leq (\beta U)^{-1} \tag{3.6}$$

and the pairing susceptibility as

$$(\widehat{p}_q, \widehat{p}_{-q}) \leq (\beta U)^{-1}. \tag{3.7}$$

Here (A, B) is the Duhamel two-point function $(A, B) = \int_0^1 \mathrm{Tr}[A^\dagger e^{t\beta H} B e^{(1-t)\beta H}]\, dt$ and $\delta\widehat{n}_q = \widehat{n}_q - \langle\widehat{n}_q\rangle$ and $p_x = c^\dagger_{x\uparrow} c_{x\downarrow}$ and $\widehat{\ }$ denotes spatial Fourier transform. Charge long range order is precluded by (3.6) while Cooper pairing is precluded by (3.7).

Although I am restricting this review to the Hubbard model, I cannot resist the temptation to mention that Theorem 1 has recently been extended [FL2] to another model—the Holstein model—in which electrons interact with a quantized phonon field instead of with each other. Again, the finite system ground state for any even number of electrons is unique and has zero spin. The method of proof of Theorem 1 has also been used by Ueda, Tsunetsugu and Sigrist [UTS] to show that the periodic Anderson model at half-filling has a singlet ground state.

This close connection between the half-filled band, repulsive Hubbard model and the antiferromagnetic Heisenberg model points to the first of our spin problems. The antiferromagnetic Heisenberg model on a hypercubic lattice, in the thermodynamic limit, has no long range order (LRO) at positive temperature in dimensions $D = 1$ or 2. This is a consequence of the Hohenberg-Mermin-Wagner theorem. The same is true for the Hubbard model as first shown by Walker and Ruijgrok [WR], then by Ghosh [GD]. Later, Koma and Tasaki [KT]proved it by a different method—that of McBryan and Spencer [MS]. As far as the ground state is concerned, the Heisenberg model has LRO for $D = 2$ and spin 1 or more per site [KLS] (i.e. $|\mathbf{S}_x|^2 = S(S+1)$ and $S \geq 1$) and it is believed to have LRO also when $S = 1/2$, which is the case of interest for us. The $D = 1$ case is believed to have no LRO in the ground state. For $D \geq 3$ there is LRO in the ground state for all $S \geq 1/2$ [KLS] and at positive temperature [DLS, KLS] for $S \geq 1$ (presumably, also for all $S \geq 1/2$). The obvious conjecture is the following.

Problem 1: *Prove that there is antiferromagnetic LRO in the half-filled band, repulsive Hubbard model on the hypercubic lattice (with $t_{xy} = 1$ for $|x - y| = 1$ and U_x = positive, finite constant) in the ground state when $D = 2$ and for positive temperature when $D \geq 3$. For which values of N will the attractive model have LRO?*

The Falicov-Kimball [FK2] model poses an analogous problem that *can be solved* affirmatively. In this model, one kinetic energy term, $K_\downarrow$, is omitted from the Hamiltonian. Although the down spins are not dynamic their locations are left arbitrary. After "integrating out" the movable particles (up-spins), an effective interaction among the fixed particles (down-spins) is left. This, then, is a classical lattice gas with a complicated interaction. It resembles an Ising (not Heisenberg) model when U is large and it can be shown [KL] to have long range order at low temperatures (and no long range order at high temperatures) in two or more dimensions—as does the Ising model.

C. The Surprising Hole

In the previous subsection we considered the half-filled band and showed a strong tendency to antiferromagnetism. The only important requirement on T was that it was real (i.e., no magnetic field acts on the orbital motion). Nagaoka [NY] made a surprising discovery about the case $U = +\infty$, but *with one hole* (i.e., $N = |\Lambda| - 1$). Thouless [TD] had a similar result a bit earlier (cf. note 7 in [NY] and the discussion on p. 47 in [LE2]) but there is little doubt that Nagaoka's presentation of this particular result is clearer, more precise and applicable to certain non-bipartite lattices such as *bcc* and *fcc*. The Thouless approach uses a Perron-Frobenius argument that appears to be restricted to bipartite lattices; for such lattices it is true that fermions behave like bosons when $U = +\infty$ and there is one hole. Nagaoka, on the other hand seems to require a regular Bravais lattice, but this is not really necessary provided *all* t_{xy} are nonpositive. The fully general result with a considerably simplified proof, was given by Tasaki [TH1].

It is usually assumed in the condensed matter literature that the t_{xy}'s are nonnegative, but there seems to be neither a compelling reason for this assumption nor many examples in which it can be verified (S. Kivelson, private communication). (For a bipartite lattice, however, one can have either sign with the help of the unitary operator $(-1)^x$ applied to *both* spin $\uparrow$ and $\downarrow$.) Notice that $t_{xy} > 0$ puts the lowest

kinetic energy at one point, namely $k = 0$, in Fourier space. The condition $t_{xy} < 0$ puts it at the edge of the Brillouin zone, and thus the lowest kinetic energy can be highly degenerate. The physical intuition is then quite different in the two cases—a fact that should not be lost sight of because of the hole-particle symmetry that holds for bipartite graphs. The proof in [TH1] shows that negative, not positive t_{xy} is the *natural mathematical assumption* for this theorem. If this upsets anyone's physical proclivity, that is a pity.

Theorem 2: *If $N = |\Lambda| - 1$, if $U_x = +\infty$ for all $x \epsilon \Lambda$, and if $t_{xy} \leq 0$ for all x, y, then the ground state has total spin $S = N/2$. This state is unique up to the trivial $(N+1)$-fold degeneracy if Λ satisfies a certain connectivity condition [TH1].*

The connectivity condition mentioned above is not stringent and it holds for all regular lattices in dimension greater than one (see also [AL]). Essentially it means that there are loops that permit nontrivial permutations of the particles.

In the case that Λ is completely translation invariant, i.e., that all vertices of Λ are equivalent, as is the case on a hypercubic lattice on a torus, a different proof of the theorem, very similar to Nagaoka's, was given by Tian [TG1] and by Trugman [TS].

The obvious next question to ask is this: *If there is more than one hole ($N < |\Lambda| - 1$) and $U = +\infty$, is the ground state totally ferromagnetic, i.e., is $S = N/2$?* There can be no simple general theorem because numerical calculation on small systems show that the answer seems to be "no" and, at the same time, no simple pattern seems to emerge. Yet there are a few theoretical results, as follows.

(i) The Nagaoka-Tian-Trugman method can be generalized for Λ = the D-dimensional hypercubic lattice with periodic boundary conditions and with $t_{xy} = t =$ nonpositive constant to show [TG2, TG3, TS, SQT1] that the completely magnetized state energy, $E(S = N/2; \Lambda)$, when compared to the actual ground state energy, $E(\Lambda)$, satisfies

$$\lim_{\Lambda \to \infty} E(S = N/2; \Lambda) - E(\Lambda) = 0 \tag{3.8}$$

in the thermodynamic limit, $\Lambda \to \infty$, when the number of holes $N_h = |\Lambda| - N$ is not too large. The best result is by Shen, Qiu and Tian [SQT1], which gives (3.8) when $N_h < |\Lambda|^\alpha$ with $0 < \alpha < 2/(D+2)$. Note that we do not divide by $|\Lambda|$ in (3.8), which thus truly represents the vanishing of a gap. The proof here is elegant and simple. However, one would expect (3.8) to hold as long as $N_h/|\Lambda| \to 0$ as $|\Lambda| \to 0$.

(ii) If there are many holes, $N_h/|\Lambda| > 0.49$ for the $D = 2$ or $N_h/|\Lambda| > 0.32$ for the $D = 3$ hypercubic lattices, and $\Lambda \to \infty$ as in (i) then

$$E(S = N/2; \Lambda) - E(S = N/2 - 1; \Lambda) \not\to 0. \tag{3.9}$$

There really is an instability of the $S = N/2$ state with respect to one spin flip. This was proved by Shastry, Krishnamurthy and Anderson [SKA]; see also [SA1]. The estimate was improved to $N_h/|\Lambda| > 0.29$ by von der Linden and Edwards [LvE]; Hanisch and Müller-Hartmann [HM] simplified the calculation (but not the estimate of 0.29).

(iii) Several authors [DW, FRDS, SA1, TB] were able to prove, for a translation invariant hypercubic lattice model, that when there are two holes the ground state energies satisfy $E(S = N/2 - 1; \Lambda) < E(S = N/2; \Lambda)$. However, assumptions have to be made about the relative lengths of the sides. Sütő [SA1] extended this to $2, \ldots, 6$ holes for a bcc lattice.

(iv) Sütő [SA2] shows, as expected, that the energy splitting needed for demagnetization is, in any case, negligible. He proves that $M(\beta, h, \rho)$, the magnetization per site in field h at density $\rho = N/|\Lambda|$ satisfies (in the thermodynamic limit) $M(\beta, h, \rho) \to \tanh(\beta h)$ as $\rho \to 1$.

The results in (ii) and (iii) are achieved with a variational calculation. The value of $E(S = N/2; \Lambda)$ is easy to find exactly because it equals the energy of spinless electrons, i.e.,

$$E(S = N/2; \Lambda) = \sum_{j=1}^{N} \lambda_j(T) \tag{3.10}$$

for any Λ and hopping matrix, T, and in which $\lambda_1(T) \leq \lambda_2(T) \leq \cdots$ are the eigenvalues of T. Thus, the hard problem is to find a good variational function with $S = N/2 - 1$, and this appears to be extraordinarily difficult. Why? No one seems to know! And why is it so difficult to treat $S = N/2 - 2$?

These results, (i)–(iii), show that one cannot expect $S = N/2$ except when $N = |\Lambda| - 1$, but one can ask the following.

Problem 2: *With $U = +\infty$, for which $\rho := N/|\Lambda|$ is it true that some (if there is more than one) ground state has $S/|\Lambda| > 0$ in the thermodynamic limit $\Lambda \to \infty$?*

This brings us to two more open problems about the $U = +\infty$ case; the first is a corollary of the second. We take a large Λ and N particles and suppose that the thermodynamic limit $\Lambda \to \infty$ with $\rho = N/|\Lambda|$ fixed is well defined. We set $S =$ spin of the ground state (the maximum such spin if there is more than one ground state) and we set $S_{\max} = N/2$. We also assume that $t_{xy} \geq 0$ for all x and y. Then

Problem 3: *Prove or disprove that*

$$\lim_{\rho \to 0} \lim_{\Lambda \to \infty} S/S_{\max} = 0. \tag{3.11}$$

Problem 4: *Does there exist some number $\rho_c > 0$ such that*

$$\lim_{\Lambda \to \infty} S/S_{\max} = 0 \quad \text{for all } \rho < \rho_c? \tag{3.12}$$

The requirement that $t_{xy} \geq 0$ is important. As we shall see in Sect. D, Mielke's work shows that there can be nice, periodic lattices in any dimension (such as the kagome lattice in two-dimensions) for which $S = S_{\max}$ for all $\rho < \rho_c$ with $\rho_c > 0$, thereby contradicting (3.11) and (3.12). To achieve this, however, one needs $t_{xy} \leq 0$. Perhaps (3.11) and (3.12) hold in the case $t_{xy} \leq 0$ if we replace "maximum such spin" by "average of such spins", because Mielke's and Tasaki's examples have highly degenerate ground states with spins ranging from 0 to $N/2$.

Closely related in spirit to Theorem 2, but with an interesting, different proof, is the result of Chakravarty, Chayes and Kivelson [CCK]. They start with a half-filled band, $N = |\Lambda|$, and U large. Then they add or subtract one or two particles, and define $E_n := E(N = |\Lambda| + n)$ for $-2 \leq n \leq +2$. They then define

$$\Delta_e = 2E_1 - E_2 - E_0$$

$$\Delta_h = 2E_{-1} - E_{-2} - E_0. \tag{3.13}$$

The interpretation of Δ_e is as a 2-particle binding energy, while that of Δ_h is as a 2-hole binding energy. The picture of Δ_e, for example, is that given two very large

systems at half-filling, and given two extra electrons, is it energetically favorable to add the two electrons to one system ($\Delta_e > 0$), or is it favorable to add one electron to each system ($\Delta_e < 0$)? The former, $\Delta_e > 0$, connotes **pair binding**.

It is pointed out in [CCK] that $\Delta_e \leq 0$ and $\Delta_h \leq 0$ when $U = 0$, but they quote numerical studies showing that $\Delta_e > 0$ and $\Delta_h > 0$ for some U and some Λ. They prove, however, that in the limit $U \to \infty$, $\Delta_e \leq 0$ if all t_{xy} are nonnegative and $\Delta_h \leq 0$ if all t_{xy} are nonpositive. For a bipartite graph the sign does not matter (as long as all t_{xy} are positive or all are negative), and thus $\Delta_e \leq 0$ and $\Delta_h \leq 0$ in this case. They interpret this result to mean that the numerical positive binding results are only an intermediate U phenomenon but, strictly speaking, the (unlikely) alternatives $\Delta_e = 0$ and $\Delta_h = 0$ in their theorems would first have to be eliminated.

D. Another Path to Ferromagnetism

The one-hole, $U = +\infty$ model is not the only one known to have *saturated* ferromagnetism (i.e., $S = N/2$). Mielke [Mi1] and later Tasaki [TH2] and then both [MT] found interesting, but very special models with this property.

The basic idea is to find a graph Λ and a hopping matrix T such that the lowest eigenvalue of T (call it λ_0) is highly degenerate; in fact we want the degeneracy to be at least N and, to be interesting, we want that to be of the order of $|\Lambda|$. Let N_0 denote the degeneracy of this lowest eigenvalue and denote the space of these eigenfunctions by $\mathcal{H}_0$. If $U_x \geq 0$ for all $x \in \Lambda$, it is easy to see that if $N = N_0$ then

(i) There is a ground state having $S = N_0/2$.

(ii) The state is simply a determinant formed from the N_0 vectors in $\mathcal{H}_0$ and its energy is $N_0\lambda_0$.

(iii) The ground state is unique if certain additional conditions (known to be optimal) are met [Mi1].

If $N < N_0$ the ground state manifold will contain at least one state with $S = N/2$, but perhaps others as well (see [Mi1]).

A comparison with Theorem 1 is interesting, but it is not clear whether or not it is misleading. Note that the $S = \big||A| - |B|\big|/2$ result there for a bipartite graph and a half-filled band was somehow related to the $\big||A| - |B|\big|$-fold degeneracy of the zero-mode of T. Thus, a common feature is degeneracy, and it is often said that itinerant ferromagnetism is associated with atomic or kinetic energy degeneracy. But there are also important differences:

(i) The spin in Theorem 1, while it might be proportional to $|\Lambda|$, is not $N/2 = |\Lambda|/2$.

(ii) No fine tuning of T or of Λ was needed for Theorem 1. All that was needed was the bipartite structure, the positivity of the U_x's and the reality of the t_{xy}'s.

Mielke's way of achieving the degeneracy N_0 is to start with some graph G and then to set $\Lambda = L(G)$, the **line graph of G**, which is defined as follows. Make a mark in the center of every edge of G; those marks will be the sites of $L(G)$. Two sites are connected by an edge in $L(G)$ if the two edges of G on which they reside have a G-site in common. Note that $L(G)$ is never bipartite, except for the trivial case of a ring. A well known example of a line graph is the kagome lattice. (Incidentally, kagome is not a person—it is a pattern of woven bamboo.)

The hopping matrix T is defined to be $-t < 0$ on every edge of $\Lambda = L(G)$. Not only is there a restriction on the magnitude of t_{xy} but we see, once again, that negative t_{xy} is the natural sign—as it is for Theorem 2.

Of course, as Mielke and Tasaki note, and as is also true in Theorem 2, one can convert positive t_{xy} into negative t_{xy} by a hole-particle transformation on both spin $\uparrow$ and spin $\downarrow$. This does not alter the interaction or the total spin, S, but it changes N into $N' = 2|\Lambda| - N$. For positive, t_{xy}, then, we can transform to the negative t_{xy} situation and conclude that $S = N'/2$ when $N' \leq N_0$. This translates into $S = |\Lambda| - N/2$ when $N \geq 2|\Lambda| - N_0$ (and not $\leq$). This construction would yield saturated ferromagnetism, $S = N/2$, only at $N = |\Lambda|$ (half-filled band), provided it were possible to achieve $N_0 \geq |\Lambda|$; this is clearly impossible (unless $T = 0$), so the positive t_{xy} choice does *not* yield the desired saturated ferromagnetism. However, it is still possible to have unsaturated ferromagnetism, i.e. $1 > 2S/N \neq 0$ in the thermodynamic limit. By taking $N = 2|\Lambda| - N_0$ and $S = |\Lambda| - N/2$ we have $2S/N = N_0/(2|\Lambda| - N_0)$. (One *can* reasonably argue, however, that the condition $S = |\Lambda| - N/2$ *is indeed* saturated ferromagnetism because this value of the spin is the maximum possible one when $N > |\Lambda|$, given the constraints of the sytem and given the Pauli principle. The system is constrained by allowing only a limited number of states for the electrons, i.e., two per site. I leave the semantic resolution to the reader.)

The homology of G determines $\mathcal{H}_0$ in a simple way. Pick any closed, self avoiding path in G of even length. This path corresponds, in an obvious way, to a closed path, P, of the same length in $L(G)$. If, now, we take the vector $\phi(x) = 0$ for x not a vertex of P and $\phi(x) =$ alternately $+1$ and -1 as we traverse the vertices of P, we see at once that ϕ is an eigenvector with eigenvalue $-2t$. It is also not hard to prove that $-2t$ cannot be improved, i.e., $\lambda_0 = -2t$. Moreover, this construction yields all of $\mathcal{H}_0$.

In [TH2, MT] essentially the same result as Mielke's (with similar requirements on T) is achieved, but with certain decorated lattices with next nearest neighbor hoppings. The ferromagnetism of [TH2, MT] is shown to be stable under small change of the electron density, by using a "grand canonical ensemble" with a fixed electron density. It is also proved that there is a transition to a paramagnetic phase as one decreases the electron density. Thus (3.11) and (3.12) (with S replaced by its grand canonical average) are proved for these special graphs.

In all cases, the eigenvectors in $\mathcal{H}_0$ can all be taken to have compact support, i.e., each $\phi(x)$ vanishes except on a finite set of sites of Λ, and each such set is independent of Λ once Λ is large enough to include the set. This property leads to the result [MT] that the effective Hamiltonian, in a suitable subspace of states that includes the ground states, can be written exactly as a Heisenberg Hamiltonian.

IV. THE FLUX PHASE PROBLEM

Very little seems to be known rigorously about the effect of a magnetic field on the orbital motion, that is, if we set

$$t_{xy} = |t_{xy}| \exp[i\theta_{xy}], \qquad \theta_{xy} = \int_x^y A \cdot ds \tag{4.1}$$

for some vector potential A. The spin of the ground state might well change. The known proofs of Theorems 1 and 2 fail when $A \neq 0$. If, indeed, the spin of the ground state changes then we have a new kind of "magnetic field—spin" interaction, brought about by the Pauli exclusion principle. Indeed, something similar is discussed in the one-dimensional context in [FK1].

Whether or not the spin changes, it is certain that the energy can often be lowered by a magnetic flux. [The flux through a circuit of n sites is the argument of the product of the t's as the circuit is traversed, i.e. $arg(t_{12}t_{23}\cdots t_{n1})$.] If $N = 1$ the optimum choice is zero flux—this is the diamagnetic inequality. The remarkable fact is that when the density $N/|\Lambda|$ is positive, a nonzero flux can lower the energy, thereby violating the diamagnetic inequality. Many theoretical and numerical investigations over the past six years have led to the conjecture that for a square, planar lattice the optimum flux is $\pi N/|\Lambda|$ in each square plaquette when $U = 0$. (For a survey of this question and for some rigorous results about it, see [LL2].) Thus, the half-filled band is said to give the maximum possible violation of the diamagnetic inequality; the effect is entirely due to the Pauli principle, for there are no Zeeman terms here.

The conjecture has been proved [LE3] for $N = |\Lambda|$, even for *arbitrary* dimension, D, and even with a Hubbard type point interaction of any sign (more generally, a reflection positive potential). What is required is that Λ be hypercubic and that in $D-1$ directions we have *(i)* an even number of sites, *(ii)* periodic boundary conditions, *(iii)* the $|t_{xy}|$'s are reflection symmetric with respect to all midplanes perpendicular to these directions. (The hexagonal planar lattice is a special case.) See [LE3] for more details and an illustrative figure.

Theorem 3: *With the conditions on Λ stated above, and $N = |\Lambda|$, the optimum flux for the ground state and for the positive temperature state is π in each square face of the hypercubic lattice.*

Remarks: (1). Since flux π can always be achieved with real t_{xy}'s, it follows from Theorem 1 that the ground state has spin zero. Thus, the *optimum* magnetic field does not change the spin of the ground state in this particular case.
(2). The theorem can be generalized to more complicated interactions and to gauge fields more complicated than $U(1)$, e.g., $SU(2)$ fields. $SU(2)$ electron symmetry is also not required, so the theorem holds, e.g., for the Falicov-Kimball model.

Problem 5 (revised): *Solve the flux phase problem for $U \neq 0$ (or even for $U = 0$) for a less than half-filled band on a square lattice.*

V. UNIFORM DENSITY THEOREM

The hole-particle transformation has remarkable consequences for the Hubbard model on a bipartite graph with a half-filled band, $N = |\Lambda|$. The ideas given below are well known to chemists—less so to physicists. They go back to Coulson and Rushbrooke [CR] for the $U = 0$ case, and to MacLachlan [MA] who generalized them to many interacting models—including the Hubbard model as a special case. A simplified proof together with an extension to models involving explicity spin-spin interactions (such as the $t - J$ model), and to the Falicov-Kimball model, is given in [LLM].

The results apply equally to three cases: (a) The canonical Gibbs state with $N = |\Lambda|$; (b) The grand-canonical Gibbs state with zero chemical potential; (c) The ground state with $N = |\Lambda|$ and which is defined, in case of degeneracy, to be the $\beta \to \infty$ limit of the canonical Gibbs state. The one-body density matrix $\rho_\sigma(x, y)$ is the expectation value of $c^\dagger_{x\sigma}c_{y\sigma}$ in the state in question.

Theorem 4: *For a half-filled band on a bipartite lattice, the one-body density matrix for each of the above states satisfies (for each* $\sigma = \uparrow$ *or* $\downarrow$*).*

$$\rho_\sigma(x,y) = \tfrac{1}{2}\delta_{xy} \qquad \text{if } x,y\epsilon A \text{ or } x,y\epsilon B. \tag{5.1}$$

If $x\epsilon A$ and $y\epsilon B$, nothing simple can be said. Note that the theorem does *not* require T to be real, and is thus one of the few theorems that applies to complex t_{xy}. However, a true, physical magnetic field would also act on the electron spins and thereby vitiate the hole-particle symmetry needed for the proof.

The complex case is a bit subtle, for it uses more than just a hole-particle transformation (call it W). It also utilizes the nonlinear antiunitary map J that maps a vector ψ, considered as a polynomial in the $c^\dagger_{x\sigma}$'s applied to the vacuum, into the vector ψ^* corresponding to the polynomial with complex conjugate coefficients. While J is nonlinear, JKJ is linear when K is any linear operator, and $TrJKJ = (TrK)^*$. The antiunitary $Y = JW$ satisfies $Y = JW = WJ$ (and hence $Y^2 = \mathbf{1}$) and $Yc_{x\sigma}Y = Wc_{x\sigma}W$. Most important is the invariance of the Hamiltonian, $YHY = H$, which replaces the hole particle invariance, $WHW = H$, which fails for complex T.

What is the significance of this result? It seems to contradict the conjecture in Problem 1 that there can be antiferromagnetic, i.e., staggered, LRO. Such an ordering can occur only in the thermodynamic limit and it has the property that for every state with ordering $\uparrow\downarrow\uparrow\downarrow\cdots$ there is a state with ordering $\downarrow\uparrow\downarrow\uparrow\cdots$. The point about Theorem 4, applied to the thermodynamic limit, is that for every state with ordering there is an equally good state (obtained by changing boundary conditions) with the opposite ordering, and on the average each site will have the same density for each spin value. In other words, *there is no way to adjust the potentials* U_x *or the hopping matrix* t_{xy} *in a clever way so as to enhance the occupation of certain sites* — in a manner independent of boundary conditions. This stability is remarkable and, although it is not true for real materials, the theorem hints at some kind of remnant stability that might transcend the overly idealized assumptions needed for its proof.

Problem 5: *Is there any residue of (5.1) when* $N \neq |\Lambda|$?

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Flux Phase of the Half-Filled Band

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The conjecture is verified that the optimum, energy minimizing, magnetic flux for a half-filled band of electrons hopping on a planar, bipartite graph is π per square plaquette. We require *only* that the graph has periodicity in one direction and the result includes the hexagonal lattice (with flux 0 per hexagon) as a special case. The theorem goes beyond previous conjectures in several ways: (1) It does not assume, *a priori*, that all plaquettes have the same flux (as in Hofstadter's model). (2) A Hubbard-type on-site interaction of any sign, as well as certain longer range interactions, can be included. (3) The conclusion holds for positive temperature as well as the ground state. (4) The results hold in $D \geq 2$ dimensions if there is periodicity in $D-1$ directions (e.g., the cubic lattice has the lowest energy if there is flux π in each square face).

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The flux phase conjecture states that the ground state (g.s.) energy minimizing magnetic flux through a square, planar lattice on which free electrons hop is π per plaquette when the electron filling factor is $\frac{1}{2}$ [1–4]. (Zeeman terms are excluded.) This conjecture, along with extensions to positive temperature, higher dimensional geometries, and allowance for some electron-electron interactions, will be proved here.

If the sites of the lattice are interpreted as atoms in a solid then flux π would correspond to magnetic fields available only on neutron stars. The significance of the flux phase is thus not primarily as a literal interpretation in terms of physical magnetic fields. One interesting interpretation concerns mean field calculations connected with superconductivity. The main interest, however, in the author's view, is that it shows that diamagnetism (which states that the optimal flux is zero—and which is correct when the electron density is very small) can be reversed when the electron density is high. Indeed, it can be maximally reversed, as in this case (since flux on a lattice is determined only modulo 2π). Thus, there is a peculiar, nonintuitive, and poorly understood effect of the Pauli principle on the way in which orbital motion interacts with magnetic fields. It has been studied extensively [5–13]. See [10] for some history.

To define things precisely, we start with a general *finite graph* Λ, which is a collection of $|\Lambda|$ sites and certain bonds denoted by xy with x and y in Λ and $x \neq y$. A positive weight $|t_{xy}| = |t_{yx}|$ is specified in advance for each bond. By convention $t_{xx} = 0$. The hopping amplitude is then $t_{xy} = |t_{xy}| \exp[i\phi(x,y)]$, with $\phi(x,y) = -\phi(y,x)$ for Hermiticity, and the problem is to find the numbers $\phi(x,y)$ that minimize the total electronic ground state energy (when $\beta = 1/kT = \infty$) or free energy (when $\beta < \infty$). $\phi(x,y)$ is the integral of the vector potential, from x to y.

A *circuit* in Λ is a sequence of points $x_1, x_2, \ldots, x_n, x_1$ with $t_{x_i x_{i+1}} \neq 0$ for all i. The *flux* through this circuit is $\sum_{i=1}^{n} \phi(x_i, x_{i+1}) \pmod{2\pi}$. It is a fact [10] that the spectrum of the Hermitian matrix $T = \{t_{xy}\}_{x,y\in\Lambda}$ depends on the ϕ's *only* through the fluxes. This is also true of the Hamiltonians below. No *a priori* assumption is made that the flux need be the same in all plaquettes; indeed, the flux is not even assumed to be the same for up- and down-spin electrons. We allow different $|t_{xy}|$'s and $\phi(x,y)$'s for the up- and down-spin electrons. We denote these by $T^{\uparrow}$, $T^{\downarrow}$. Thus, our results apply to the Falicov-Kimball model (where $T^{\downarrow} = 0$), for example.

The *electronic kinetic energy operator*, in second-quantized notation, is

$$K = -\sum_{x,y\in\Lambda} t^{\uparrow}_{xy} c^{\dagger}_{x\uparrow} c_{y\uparrow} + t^{\downarrow}_{xy} c^{\dagger}_{x\downarrow} c_{y\downarrow}. \tag{1}$$

The c's satisfy the fermion anticommutation relations $\{c^{\dagger}_{x\sigma}, c_{y\tau}\} = \delta_{xy}\delta_{\sigma\tau}$, $\{c_{x\sigma}, c_{y\tau}\} = 0$. The electron number is $N = N_{\uparrow} + N_{\downarrow}$ and $N_{\sigma} = \sum_{x\in\Lambda} n_{x\sigma}$ with $n_{x\sigma} = c^{\dagger}_{x\sigma} c_{x\sigma}$. If the Hamiltonian H equals K, then the ground state energy E_0 would be $E_0 = \sum_{\lambda<0} \lambda(T^{\uparrow}) + \sum_{\lambda<0} \lambda(T^{\downarrow})$, i.e., the sum of the negative eigenvalues, $\lambda(T)$, of the matrices $T^{\uparrow}$ and $T^{\downarrow}$.

For *bipartite graphs* (i.e., $\Lambda = A \cup B$, $A \cap B = \varnothing$ and $t_{xy} = 0$ unless $x \in A$, $y \in B$ or $x \in B$, $y \in A$) E_0 is achieved when $N = |\Lambda|$, and hence the appelation half-filled band, since $0 \leq N \leq 2|\Lambda|$ in general. In the Hubbard model $H = K + W^0$,

$$W^0 = \sum_{x\in\Lambda} U_x \left(n_{x\uparrow} - \tfrac{1}{2}\right)\left(n_{x\downarrow} - \tfrac{1}{2}\right), \tag{2}$$

but we can also add certain longer range density-density interactions, W^d and spin-spin interactions W^s to be specified later, of the form (with $w^k_{xy} = w^{k*}_{xy} = w^k_{yx}$, $k = d, 1, 2, 3$, and S^j being Pauli matrices)

$$W^d = \sum_{x,y\in\Lambda} w^d_{xy} (n_{x\uparrow} + n_{x\downarrow} - 1)(n_{y\uparrow} + n_{y\downarrow} - 1),$$

$$W^s = \sum_{j=1}^{3} \sum_{x,y\in\Lambda} \sum_{\sigma,\tau,\mu,\lambda} w^j_{xy} (c^{\dagger}_{x\sigma} S^j_{\sigma\tau} c_{x\tau})(c^{\dagger}_{y\mu} S^j_{\mu\lambda} c_{y\lambda}). \tag{3}$$

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W^0, W^d, and W^s are invariant under the unitary hole-particle (h-p) transformation τ, with $\tau c_{x\sigma}\tau^{-1} = c^\dagger_{x\sigma}$. The kinetic energy operator with complex T's satisfies

$$\tau K(T^\dagger, T^\dagger)\tau^{-1} = K(-T^{t*}, -T^{t*}), \qquad (4)$$

where T^* denotes the complex conjugate matrix $t_{xy} \to t^*_{xy} = t_{yx}$.

The grand-canonical partition function of our system, which we want to maximize, is $Z = \mathrm{Tr}\exp[-\beta H]$ at inverse temperature β. By h-p symmetry, $\langle N\rangle \equiv \mathrm{Tr}Ne^{-\beta H}/Z$ is $|\Lambda|$, which is the half-filled band. The $\beta \to \infty$ limit is discussed at the end.

Henceforth, all graphs will be bipartite, in which case all elementary circuits contain an even number of sites and bonds. The original flux phase conjecture is that when $H = K$, $N = |\Lambda|$, and Λ is planar the optimum choice of fluxes is π in every circuit containing 0(mod4) sites and 0 in circuits with 2(mod4) sites.

Several cases of this were proved in [9,10] and it was pointed out in [10] that the conjecture cannot always hold for *arbitrary* values of $|t_{xy}|$. It depends on Λ. Despite this caveat, however, it was proved in [10] that $\ln[\det(T^2)] = \sum_j \ln[\lambda_j(T)^2]$ is maximized when the fluxes accord with the conjecture. This is true for an *arbitrary* bipartite, planar graph with *arbitrary* $|t_{xy}|$'s. (On any bipartite graph, the nonzero eigenvalues of T come in opposite pairs $\lambda, -\lambda$.)

The *generalized flux phase conjecture* is that the above choice is also optimal for $H = K + W^0 + W^d + W^s$ and for all $\beta \le \infty$. We shall prove this here for graphs that have a certain periodicity. The usual square lattice with periodic boundary conditions is included. The result holds also for higher dimensional, nonplanar graphs. The type of graphs Λ considered here is illustrated in Fig. 1 for the planar case. Λ is wrapped on a cylinder, i.e., the sites at the right end are identified with the sites on the left. The $|t_{xy}|$'s on the vertical edges must be periodic, i.e., they are allowed to vary in an arbitrary way along each column, but all the columns must be identical. The horizontal $|t_{xy}|$'s can also vary as we move vertically but they are only required to have period 2 in the horizontal direction, i.e., every *second* column of horizontal edges must be the same. Thus, if we erase the horizontal edges 1, 3, 5, etc., from every second column and if we erase edges 2, 4, 6, etc., from the remaining columns in between, the hexagonal lattice is obtained. Our result includes this case, and flux π in each (imaginary) square then implies flux 0 in each hexagon. Octagons, decagons, etc., can also be included provided periodicity 2 is maintained. We can, if we wish, insert vertical edges connecting the bottom row to the top row, as indicated by the vertical arrows in Fig. 1. Λ will no longer be planar, but that does not matter.

An easier way to state the periodicity requirements is to cut Λ at the two dashed lines, called P in Fig. 1. The two half cylinders (as well as the $|t_{xy}|$'s on the edges) are

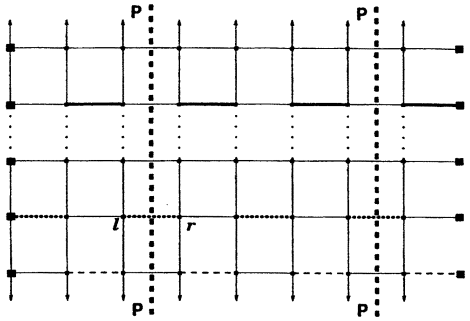

FIG. 1. Typical 2D lattice with horizontal periodic boundary conditions (left boxes = right boxes). Different bond weights illustrate the requirement of horizontal periodicity 2. Dashed lines (P) are a reflection plane. A generic left-right pair of sites is indicated by l, r.

required to be mirror images of each other. The $|t_{xy}|$'s on the edges that intersect the dashed lines are arbitrary because each is its own mirror image. We then say that $|T|$ is *reflection symmetric* with respect to the cutting lines, P, through the bonds. Our theorem says that the optimum flux is then π for those squares containing the cutting lines. If the $|t_{xy}|$'s are reflection symmetric with respect to (w.r.t.) *every* choice of cutting lines—which is equivalent to the above periodicity requirement—then flux π will be optimal in *every* square of Λ.

The periodicity of the $|t_{xy}|$'s mentioned above is *not* needed for the theorem below. Only reflection symmetry is needed. The periodicity comes in when we wish to insure flux π in *every* plaquette of Λ. This is achieved by repeated reflection in hyperplanes in the standard way [14,15]; indeed, one can easily derive the usual chessboard estimates [14].

In fact Λ could be built in a similar way out of D-dimensional (hyper)cubes instead of squares. Cutting lines become cutting $(D-1)$-dimensional hyperplanes, and reflection symmetry is generalized in an obvious way. Our theorem will then state that the optimal flux in each two-dimensional square plaquette of the (hyper)cubic lattice is π in every plaquette cut by the hyperplanes. As in the $D = 2$ case, flux π will be optimal in *every* plaquette if we have periodicity in $D-1$ directions.

Returning to the two-dimensional situation (with obvious generalization to $D > 2$) we require only that the U_x's in W^0 be constant in the horizontal direction (as are the $|t_{xy}|$'s on vertical edges). As for w^k_{xy} in W^d and W^s, they are required to be reflection positive for reflection in vertical planes (the dashed lines, P, in Fig. 1), as explained below. The inclusion of W^d and W^s is mainly for completeness and nothing essential will be lost by setting $W^d = W^s = 0$.

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In general, a Hamiltonian can be written (with respect to a cutting hyperplane, P) as

$$H = H_L + H_R + H_{\text{int}}, \tag{5}$$

where H_L is all the terms involving sites in the left half cylinder, H_R involves right half-cylinder sites and H_{int} involves both. The subscripts L, R, and int will also be used for the separate pieces, e.g., K_L, K_R, K_{int}, etc. Associated with the left Hamiltonian H_L is a right Hamiltonian, $\Theta(H_L)$, which is obtained from H_L by three steps: *the unitary transformation $\mathcal{R}$ generated by geometric reflection through the plane P; hole-particle transformation τ; and complex conjugation* $*$. $\Theta(H_L) = [\tau\mathcal{R}(H_L)\tau^{-1}]^*$. This notion of *operator reflection* can be applied to any operator A_L in the left algebra (i.e., A_L is a polynomial in the operators $c_{x\sigma}$, $c^\dagger_{x\sigma}$ with x in the left half cylinder). In particular, $\Theta(c_{l\sigma}) = c^\dagger_{r\sigma}$. A similar definition holds for the left Hamiltonian $\Theta(H_R)$ and, clearly, $\Theta(\Theta(H_L)) = H_L$. Note, from (4), that $\Theta(K_L) = -\mathcal{R}(K_L)$, $\Theta(W^\alpha) = \mathcal{R}(W^\alpha)$, $\alpha = 0, d, s$.

Reflection positivity of w_{xy} means that it is symmetric under reflections and, for x in the left and y in the right half cylinder, w_{xy} can be written as a sum (or integral) of functions of the form $a(x)a(\mathcal{R}y)^*$. In other words, W^d_{int}, W^s_{int} are sums (or integral) of operators of the form $-A_L\Theta(A_L)$, where the $(-)$ in W^d_{int} comes from $\tau(n_{x\uparrow} + n_{x\downarrow} - 1)\tau^{-1} = 1 - n_{x\uparrow} - n_{x\downarrow}$, and similarly for W^s_{int}. An important example is $w_{xy} = w > 0$ if x, y are nearest neighbors, $w_{xy} = 0$ otherwise. Such a W^s is antiferromagnetic; see [14].

Concerning K_{int}, we note that it is generally not invariant under the three operations. However, with l and r denoting a generic left and right image pair cut by P, we are at liberty to choose $\phi(l, r) = 0$, i.e., $t_{lr} = |t_{lr}| \geq 0$, and we do so. (Note: to simplify the notation the symbols, $\uparrow$ and σ, will not be indicated.) This is so because a simple gauge transformation $c_r \to \exp[-i\phi(l, r)]c_r$ makes $t_{lr} > 0$ without changing any fluxes. No circuits are involved. This choice of phase for t_{lr} is only a convention, for it does not change any physics, but it is important for (6) and (7) below.

With the foregoing convention for H_{int}, the Hamiltonian is said to be *reflection symmetric* if $\Theta(H_L) = H_R$. The flux π theorem will be a corollary of the following lemma.

Lemma (reflection positivity).—With H as a given in (5) with respect to some hyperplane P, assume that K_{int} satisfies the above positivity convention. Assume also that W^d_{int} and W^s_{int} are reflection positive. Then, for each $\beta \geq 0$ and with H_{int} fixed,

$$Z(H_L, H_R)^2 \leq Z(H_L, \Theta(H_L))Z(\Theta(H_R), H_R), \tag{6}$$

where $Z(H_L, H_R) \equiv \text{Tr}\exp[-\beta H]$. Moreover, if $H_R = \Theta(H_L)$ and if A_L (A_R) is any even operator in the left (right) algebra (e.g., A_L is a sum of monomials in $c^\#_{x\sigma}$ of even degree) then

$$|\text{Tr}A_L A_R e^{-\beta H}|^2 \leq \text{Tr}A_L\Theta(A_L)e^{-\beta H}\text{Tr}\Theta(A_R)A_R e^{-\beta H}. \tag{7}$$

Proof: Use the Lie-Trotter formula to approximate $e^{-\beta H}$ as a product of $M \gg 1$ factors $V = V_{\text{int}}V_L V_R$, i.e., $e^{-\beta H} = \lim_{M\to\infty} V^M$, where $V_{\text{int}} = 1 - \beta H_{\text{int}}/M$, $V_L = \exp[-\beta H_L/M]$, $V_R = \exp[-\beta H_R/M]$. Notice that V_L contains only even polynomials in the $c^\#$'s, and so V_L commutes with every right operator (including odd operators). Likewise, V_R commutes with all left operators.

If the M factors of V_{int} are multiplied out we obtain for V^M a sum of terms, each having the form $X = a_1 V_L V_R a_2 V_L V_R a_3 V_L V_R \cdots a_M V_L V_R$ and each a_i has one of three forms: (i) $A_L\Theta(A_L)$, with A_L an even operator or (ii) $c^\dagger_l c_r$ or (iii) $-c_l c^\dagger_r$. Our strategy is to move all the left operators to the left *without* changing the order either of the left operators among themselves or the right operators. The operators A_L commute with all the right operators and cause no difficulty. The difficult point is that the $c^\#_l$ operators have to move through the $c^\#_r$ operators to their left, and each such move gives rise to a -1 factor.

I claim that either $\text{Tr}X = 0$ or else the number of -1 factors is even. To see this note that by particle conservation (and the particle conserving nature of V_L and V_R) the number of $c^\dagger_l c_r$ factors must equal the number of $c_l c^\dagger_r$ factors if $\text{Tr}X \neq 0$. Call this common number J. The number of -1 factors is independent of the order of these $2J$ factors and their order relative to the $A_L\Theta(A_L)$ factors. The first $c^\#_l$ must move through zero $c^\#_r$'s. The second $c^\#_l$ moves through one $c^\#_r$, etc. Thus, the number of -1 factors is $0 + 1 + 2 + \cdots + (2J - 1) = J(2J - 1)$. On the other hand, each $c_l c^\dagger_r$ term carries a -1 factor and there are J of these. Altogether there are $J + J(2J - 1) = 2J^2 = 0(\text{mod}2)$ factors of -1, as claimed.

In brief, X can be brought into the form $X = X_L X_R$ with X_L and X_R even operators. Since $\text{Tr}\mathbf{1} = 4^{|\Lambda|}$, we have $4^{|\Lambda|}\text{Tr}X = \text{Tr}X_L\text{Tr}X_R$. Moreover, $(\text{Tr}X_L)^* = \text{Tr}\Theta(X_L)$ and thus $|\text{Tr}X_L|^2 = \text{Tr}X_L\Theta(X_L)$. Now, denoting the various X's by X^α, we have $|\text{Tr}V^M|^2 = |\sum_\alpha \text{Tr}X^\alpha|^2 = 4^{-2|\Lambda|}|\sum_\alpha \text{Tr}X^\alpha_L\text{Tr}X^\alpha_R|^2 \leq 4^{-2|\Lambda|}\sum_\alpha |\text{Tr}X^\alpha_L|^2\sum_\alpha |\text{Tr}X^\alpha_R|^2 = \sum_\alpha \text{Tr}X^\alpha_L\Theta(X^\alpha_L)\sum_\alpha \text{Tr}X^\alpha_R\Theta(X^\alpha_R) \to Z(H_L, \Theta(H_L))Z(H_R, \Theta(H_R))$. (7) is obtained in the same way. Q.E.D.

Theorem (flux π is optimal).—Assume the $|t^{l,l}_{xy}|$ are reflection invariant w.r.t. P. Assume also that $\Theta(W^\alpha_L) = W^\alpha_R$ and W^α_{int} is reflection positive, $\alpha = 0, d, s$. Then Z is maximized by putting flux π in each square face of Λ that intersects P.

Proof: We make the gauge transformation above so that K_{int} has $t_{lr} = |t_{lr}|$. From (6), we have that when H_L, H_R is optimal, so is H_L, $\Theta(H_L)$ and $\Theta(H_R)$, H_R. But the statement $K_R = \Theta(K_L)$ implies the flux π condition by (4). Q.E.D.

Remarks: (i) It is interesting to note that (6) can also be used to show that when the fluxes are fixed at π and one varies over the $|t_{xy}|$, the lowest energy is attained

in a reflection symmetric configuration of $|t_{xy}|$. A one-dimensional version of the lemma was proved and used in [16] to study the Peierls instability for the Hubbard model on a ring.

(ii) The lemma and theorem say that flux π for $T^{\uparrow}$ and $T^{\downarrow}$ is optimal. If we fix $\phi^{\downarrow}(x,y)$, we are then free to choose $\phi^{\uparrow}(x,y) = \phi^{\downarrow}(x,y)$, since any other choice with flux π differs from $\phi^{\downarrow}(x,y)$ by a trivial gauge transformation, $c_{x\downarrow} \to e^{i\mu(x)}c_{x\downarrow}$. Thus, when $|t^{\downarrow}_{xy}| = |t^{\downarrow}_{xy}|$, the minimizer can have $T^{\downarrow} = T^{\uparrow}$, thereby preserving SU(2) invariance.

(iii) To discuss the ground state we let $\beta \to \infty$. Do we get $N = |\Lambda|$ or does the g.s. belong to $N = |\Lambda| + m$ and $N = |\Lambda| - m$ with $m > 0$? In the Falicov-Kimball model, generally, the g.s. has $N = 2|A|$ and $N = 2|B|$, as the only choices [17] (but note that $2|A| = 2|B| = |\Lambda|$ in our case). In the following cases I can also prove that at least one g.s. has $N = |\Lambda|$.

First, assume reflection symmetry and positivity w.r.t. *all* hyperplanes parallel to P, so that we are now looking at a K with flux π in *every* plaquette of Λ. After a trivial gauge transformation, this condition can be realized with real T, which we assume henceforth. Next, assume $T^{\uparrow} = T^{\downarrow}$, so that SU(2) invariance holds. Third, assume $W^d = W^s = 0$, i.e., the Hubbard model. As is well known, we can then construct another set of SU(2) generators—the *pseudospin*. (See [18] and, for more details, [19].) By using the spin and pseudospin raising operators $\sum_x c^{\dagger}_{x\uparrow}c_{x\downarrow}$, $\sum_x (-1)^x c^{\dagger}_{x\uparrow}c^{\dagger}_{x\downarrow}$ [with $(-1)^x = +1$ for $x \in A$, -1 for $x \in B$], and their adjoints, one can conclude that the absolute ground state belongs to $N = |\Lambda|$ or $N = |\Lambda| \pm 1$.

Finally, to show that the g.s. has $N = |\Lambda|$, assume that either $U_x \le 0$ for all x or $U_x \ge 0$ for all x. We can then use spin-space reflection positivity [18] in *Fock space*, together with the evenness of $|\Lambda|$ in our case, to infer $N = |\Lambda|$. [This reflection positivity tells us that if a g.s. has numbers $N_{\uparrow} = \lambda$, $N_{\downarrow} = \mu$ then there are ground states with (λ,λ) and (μ,μ). Thus, if $|\Lambda| = 2m$ and $N = |\Lambda| - 1$, so that $N_{\uparrow} = m$, $N_{\downarrow} = m - 1$, then there is also an (m,m) g.s.] If all $U_x \ne 0$, the g.s. is unique [18].

Extensions: The flux phase for the half-filled band has been proved here for a large class of Hamiltonians, including the ones common in the physics literature. The proof is sufficiently simple that it obviously applies to many other models.

One generalization is to fermions with $n \ne 2$ colors, i.e., from SU(2) to SU(n).

Certain specialized forms of electron-phonon interactions can be included.

Another generalization is to SU(2) instead of U(1) gauge fields [15,20]. Thus, $t_{xy}\sum_{\sigma} c^{\dagger}_{x\sigma}c_{y\sigma}$ is replaced by $|t_{xy}|\sum_{\sigma\tau} c^{\dagger}_{x\sigma}U^{\sigma\tau}_{xy}c_{y\tau}$ with $|t_{xy}|$ given, as before, and with $U_{xy} \in$ SU(2) to be determined. [Even more generally, we can replace $t^{\uparrow}_{xy}c^{\dagger}_{x\uparrow}c_{y\uparrow} + t^{\downarrow}_{xy}c^{\dagger}_{x\downarrow}c_{y\downarrow}$ by $\sum_{\sigma\lambda\tau} c^{\dagger}_{x\sigma} \times M^{\sigma\lambda}_{x;xy}|t^{\lambda}_{xy}|M^{\lambda\tau}_{y;xy}c_{y\tau}$ where $M_{x;xy} \in$ SU(2) and $|t^{\lambda}_{xy}|$ is given; in this case the SU(2) matrix associated with xy is $U_{xy} = M_{x;xy}M_{y;xy}$.] Again, we will find that the energy is minimized by flux π in each plaquette, i.e., the product of the four matrices around a plaquette satisfies $U_{xy}U_{yz}U_{zw}U_{wx} = -1$.

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Part II

Peierls Instability

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Proof of the Peierls Instability in One Dimension

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Fröhlich and Peierls showed that a one-dimensional system with a half-filled band can lower its ground-state energy by a dimerization from period 1 to period 2. It was an open question whether or not this dimerization was exact, i.e., whether additional symmetry breaking would further lower the energy. We prove that the dimerization is exact for a periodic chain of infinitely massive, harmonically bound atoms with nearest-neighbor electron hopping matrix elements that vary linearly with the nearest-neighbor distance.

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A quarter of a century ago Frölich[1] and Peierls[2] discovered an instability in one-dimensional electron systems that has come to be called the Peierls instability. Earlier, Jones[3] used such a mechanism to explain the high diamagnetism and low conductivity of bismuth. He also used the mechanism to explain the Hume-Rothery alloys. Peierls's observation was that this dimerization always occurs in one dimension.

In a word, Frölich and Peierls note that a long chain of $2N$ atoms of total length L and $2N$ electrons (half-filled band) will not have a ground state with the "obvious" periodicity $L/2N$. They show this by constructing a trial wave function of period L/N (a dimerized state) having lower energy than the period $L/2N$ function. With $L/2N$ as one unit, we have symmetry breaking from period 1 to period 2.

Given this fact, the question arises whether the energy can be lowered further by more symmetry breaking, say to period 4 or perhaps to no periodicity at all. In this paper we prove that at least for one well-known choice of the Hamiltonian the answer is no. We prove, for all N, that the dimerized states with the lowest energy are exact ground states and are the only ground states. (The amount of dimerization is unique, although for small, odd N the dimerization can vanish, in which case the ground state is unique and has period 1.) We also show that the chemical potential is discontinuous at the half-filled band, as expected. These results were announced by Lieb.[4,5] Physical intuition notwithstanding, these results are not at all obvious, for they are true for all coupling constants and do not require the infinite-N limit. In fact, as we remark later, they are not true for certain choices of the Hamiltonian and N.

The precise formulation of the electron system we shall consider is as follows. Consider a linear chain of $2N$ atoms (with periodic boundary conditions) and let w_i ($i=1,\ldots,2N$) denote the distance from atom i to atom $i+1$ (with $2N+1\equiv 1$). If $d>0$ is the equilibrium distance and $\kappa>0$ is a measure of the stiffness, the distortion energy associated with the w_i is taken to be

$$U(\{w\})=\frac{1}{2}\kappa\sum_{i=1}^{2N}(w_i-d)^2. \tag{1}$$

Now suppose there are $2N$ (spin $\frac{1}{2}$) electrons (half-filled band) which can hop between nearest-neighbor atoms, with an amplitude $t_i=t(w_i)$ to hop from atom i to $i+1$ and from $i+1$ to i. *In this paper we consider the half-filled band.* The function $t(w)$ will be explained shortly. The ground-state energy of these $2N$ electrons is

$$K(\{w\})=2\sum_{j=1}^{N}\lambda_j(T), \tag{2}$$

where $\lambda_1\le\lambda_2\le\ldots\le\lambda_{2N}$ are the eigenvalues of the $2N\times 2N$ matrix T having matrix elements $T_{i,i+1}=T_{i+1,i}=t_i=t(w_i)$ and $T_{ij}=0$ otherwise.

The total Hamiltonian is $H(\{w\})=K(\{w\})+U(\{w\})$ and the problem is to determine the ground-state energy $E_0(2N)=\min_{\{w\}}H(\{w\})$ and the configurations $\{w\}$ that attain it.

The function $t(w)$ should be something like ae^{-cw}, but we shall adopt the linear function of Su, Schrieffer, and Heeger[6]: $t(w)=b-c(w-d)$ with $b,c>0$. (We emphasize, however, that the w_i are treated as dynamical, quantum variables in Ref. 6, whereas here they are static.)

It is well known that our problem is identical to the so-called "spin-Peierls" instability for XY interacting spin-$\frac{1}{2}$ particles. Namely, let

$$h(\{w\})\equiv 4\sum_{i=1}^{2N}\{S_i^xS_{i+1}^x+S_i^yS_{i+1}^y\}t(w_i).$$

Then the ground-state energy $e(\{w\})$ of $h(\{w\})$ is obtained by a Jordan-Wigner transformation to free fermions[7] and one finds $e(\{w\})=K(\{w\})$.

If the definition of $t(w)$ and $U(\{w\})$ are suitably changed, an "integrable system" is obtained.[8,9] However, the solution in Ref. 8 covers all electron numbers *except* the half-filled band which is the most interesting case from our point of view since it is only here that one might expect only a *partial breaking* of the symmetry from period 1 to period 2.

To state our main result we must distinguish two cases. The minimum can either be taken over all choices of $\{w_i\}$, or we can add the restriction that $\sum_{i=1}^{2N}w_i=2Nl$, where l is a constant. We will refer to these two cases as

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the variable- and fixed-length cases, respectively. For the variable-length case, which is the physical case, our results hold for all values of the parameters N, κ, b, c, and d. In the fixed-length case, N is arbitrary, but we require a restriction on the other parameters. The fixed-length constraint may be relevant for certain statistical mechanical systems in which one conventionally fixes the total "volume."

One might expect that with another $t(w)$ or another $U(\{w\})$, a similar theorem would hold, at least when κ is large enough. We were unable to prove such a theorem, and wish to point out that some restriction on the parameters is essential in general, e.g., κ being large. A simple example of $N=2$ for which the ground state does not have period 2 is to let $t(w)=1-w$ and

$$U(\{w\})=\sum_{i=1}^{4}\left\{\tfrac{1}{2}\kappa w_i^2+4w_i^4\right\},$$

with $\kappa>0$ and small. One finds that the best dimerized configuration is $w_1=w_3=W$, $w_2=w_4=0$, where W is the solution of $8W^3+\frac{1}{2}\kappa W+1=0$. For small κ, $W\approx-\frac{1}{2}$. Let $H(\epsilon)$ denote the total energy of the configuration $w_1=w_3=W$, $w_2=\epsilon$, $w_4=0$. Then $H'(0)=0$, $H''(0)=-(1-W)^{-1}+\kappa$. If κ is small, then $H''(0)<0$, and so there is a configuration whose total energy is less than that of the best dimerized configuration. This example does not prove anything about large N or large κ, but it does show that one should not try to prove too much. It is conceivable that for certain $t(w)$ and $U(\{w\})$ and large N there could be a phase transition as a function of κ from period 2 (large κ) to period 4 or no periodicity (small κ).

We define the chemical potential $\mu(m)$ to be the energy required to add the mth electron to the ground state, i.e., $\mu(m)=E_0(m)-E_0(m-1)$. Here $E_0(m)$ is defined as before except that K is replaced by $2\sum_{j=1}^{m/2}\lambda_j(T)$ for even m and by

$$2\sum_{j=1}^{(m-1)/2}\lambda_j(T)+\lambda_{(m+1)/2}(T)$$

for odd m.

Theorem.—In the variable-length case for all b, c, d, κ, and N, the only configurations that minimize H are

$$w_i=W+(-1)^i\delta \quad \text{or} \quad w_i=W-(-1)^i\delta, \tag{3}$$

with W and δ being uniquely determined by b, c, d, κ, and N. Moreover, there is a gap, i.e., there is a positive constant ϵ which depends on b, c, d, and κ, but not on N, such that for all N, $\mu(2N+1)-\mu(2N)\geq\epsilon$. In the fixed-length case the same conclusions hold provided that b, c, d, and κ satisfy

$$\kappa[b-c(l-d)]\geq c^2. \tag{4}$$

Remark: Kivelson and Heim[10] argued that $\delta>0$ for all even N, while δ can be zero for N odd. However, δ is always positive for large enough N. There is no difficulty proving these statements rigorously.

Proof: Since T is unitarily equivalent to $-T$ [the unitary operator is $(-1)^i\delta_{ij}$], we see that the sum in Eq. (2) is identical to the sum of the negative eigenvalues of T. This implies that $K=\mathrm{Tr}|T|$ since $\mathrm{Tr}T=0$. From now on we shall use $\{t_i\}$ to specify the positions of the atoms rather than $\{w_i\}$. Hence,

$$H=\frac{1}{2}g\sum_{i=1}^{2N}(t_i-b)^2-\mathrm{Tr}|T|, \tag{5}$$

with $g=\kappa/c^2$.

Let Θ_κ be the unitary operator associated with translation by k sites. Then the concavity of the square-root function implies that

$$\mathrm{Tr}|T|=\mathrm{Tr}(T^2)^{1/2}\leq\mathrm{Tr}(\langle T^2\rangle)^{1/2}, \tag{6}$$

where $\langle T^2\rangle\equiv\sum_k\Theta_kT^2\Theta_k^{-1}/2N$. It is important to note here that for a configuration satisfying (3), $\Theta_kT^2\Theta_k^{-1}=T^2$, and so the above inequality is an equality.

The nonzero matrix elements of T^2 are $(T^2)_{i,i}=t_i^2+t_{i-1}^2$ and $(T^2)_{i,i+2}=(T^2)_{i+2,i}=t_it_{i+1}$. Thus, the nonzero matrix elements of $\langle T^2\rangle$ are $(\langle T^2\rangle)_{i,i}=2y^2$ and $(\langle T^2\rangle)_{i,i+2}=(\langle T^2\rangle)_{i+2,i}=z$, where $y^2=\sum_{i=1}^{2N}t_i^2/2N$ and $z=\sum_{i=1}^{2N}t_it_{i+1}/2N$. Let Ω be the matrix whose only nonzero elements are $\Omega_{i,i+2}=\Omega_{i+2,i}=1$. Then $\langle T^2\rangle=2y^2+z\Omega$.

The distortion energy is trivially expressed in terms of y and $x=\sum_{i=1}^{2N}t_i/2N$. Combining all our results we have shown

$$H\geq\tfrac{1}{2}g2N(y^2-2bx+b^2)-\mathrm{Tr}(2y^2+z\Omega)^{1/2}. \tag{7}$$

Let $s_i=x-t_i$. Then $y^2=x^2+\sum_is_i^2/2N$, so $y^2\geq x^2$. With use of Cauchy's inequality,

$$z=x^2+\sum_is_is_{i+1}/2N\geq x^2-\sum_is_i^2/2N=2x^2-y^2. \tag{8}$$

We now consider two cases depending on whether this lower bound on z is positive or negative.

Case 1 $(2x^2-y^2\geq0)$.—Consider $\mathrm{Tr}(2y^2+z\Omega)^{1/2}$ as function of z. This function is clearly concave. Since T is unitarily equivalent to $-T$, it is also even in z. Thus, it is a decreasing function of $|z|$, so that in (7) we can replace z by $2x^2-y^2$. The resulting inequality is an equality for the dimerized configuration with $\bar{t}_i=x+(-1)^i(y^2-x^2)^{1/2}$. Furthermore, since $\sum_i\bar{t}_i=2Nx=\sum_it_i$, the total length of the configuration corresponding to $\{t_i\}$ is the same as the total length of the configuration corresponding to $\{\bar{t}_i\}$. Thus, we have shown that for any choice of $\{t_i\}$ satisfying $2x^2-y^2\geq0$, there is a configuration satisfying (3), with the same total length, whose energy is at least as low. This energy is

$$H=gN(y^2-2bx+b^2)-\mathrm{Tr}[2y^2+(2x^2-y^2)\Omega]^{1/2}. \tag{9}$$

Case 2 $(2x^2-y^2<0)$.—Since $\mathrm{Tr}(2y^2+z\Omega)^{1/2}$ is de-

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creasing in $|z|$, we can bound it from above by replacing z with 0. This yields

$$H/2N \geq \tfrac{1}{2}g(y^2-2bx+b^2)-\sqrt{2}y. \quad (10)$$

In the variable-length case we use $x^2<y^2/2$ to obtain

$$H/2N > \tfrac{1}{2}g(y^2-\sqrt{2}by+b^2)-\sqrt{2}y. \quad (11)$$

A little calculation shows that this lower bound on H is attained by the dimerized configuration $\bar{t}_i$ which alternates between 0 and $\sqrt{2}y$.

The total length of the configuration corresponding to $\{\bar{t}_i\}$ need not be the same as that corresponding to $\{t_i\}$, and so we need a separate argument for the fixed-length case. Fixing the length of the chain to be $2Nl$ is equivalent to fixing x to be $b-c(l-d)$. Recalling that $g=\kappa/c^2$, the restriction (4) is equivalent to $gx \geq 1$. This inequality and $y>\sqrt{2}x$ implies $\frac{1}{2}gy^2-\sqrt{2}y > gx^2-2x$. From (10) we then obtain

$$H/2N > gx^2-gbx+\tfrac{1}{2}gb^2-2x.$$

For the dimerized configuration $\bar{t}_i$ which alternates between 0 and $2x$ this lower bound is attained. Furthermore, the configuration corresponding to $\{\bar{t}_i\}$ has the same total length as the configuration corresponding to $\{t_i\}$. This analysis shows that for any configuration belonging to case 2, there is a configuration belonging to case 1 whose energy is lower. Hence, under the hypotheses of the theorem the minimizing configurations always belong to case 1.

We have shown that for any configuration with energy E there is a configuration satisfying (3) whose energy is at least as low as E. Thus H attains its minimum at such a configuration. It remains to be shown that H attains its minimum *only* at such configurations, that W and δ are unqiue, and that there is a gap. The following lemma, which is an improvement of inequality (6), will be used.

Lemma.—As before, let $\langle T^2\rangle$ be the average of T^2 over translations. Then

$$\mathrm{Tr}(T^2)^{1/2} \leq \mathrm{Tr}(\overbrace{\langle T^2\rangle}^{2})^{1/2} - \tfrac{1}{8}\|T\|^{-3}\mathrm{Tr}(T^2-\langle T^2\rangle)^2. \quad (12)$$

Proof: By replacing T by $T/\|T\|$, we may assume $\|T\|=1$. We claim that the function $A \to \mathrm{Tr}A^{1/2} + \frac{1}{8}\mathrm{Tr}A^2$ is concave on the set of operators A with $0 \leq A \leq 1$. To prove the claim, it suffices to show that $f(x)=x^{1/2}+\frac{1}{8}x^2$ is concave on [0,1], which is trivial. The argument is now the same as in (6) with the additional remark that $\mathrm{Tr}(T^2-\langle T^2\rangle)^2=\mathrm{Tr}(T^4-\langle T^2\rangle^2)$. Q.E.D.

By using the lemma in place of inequality (6), we see that for any configuration at which H attains its minimum we have $\mathrm{Tr}(T^2-\langle T^2\rangle)^2=0$. This implies that $T^2=\langle T^2\rangle$, which implies that the configuration satisfies (3).

We must show that W and δ are unique. For such configurations H equals the right-hand side of (9), which we think of as a function of $X=x^2$ and $Y=y^2$. It is *strictly* jointly convex in X,Y, and so has a *unique* minimum over the convex region $0 \leq X \leq Y$ (variable-length case) and over the region $Y \geq X$, X fixed (fixed-length case). There are two configurations corresponding to this unique minimum unless $x^2=y^2$, in which case there is only one configuration and $\delta=0$.

To complete the proof of the theorem we must show that there is a gap. For a configuration satisfying (3) the spectrum of T may be explicitly computed. One finds that it has a gap between the $(2N)$th and $(2N+1)$th eigenvalues. However, this does not by itself imply that the system has a gap because the configuration that minimizes H for $2N-1$ or $2N+1$ electrons need not be the configuration that minimizes H for $2N$ electrons.

Recall that $E_0(2N-1)$, $E_0(2N)$, and $E_0(2N+1)$ are the ground-state energies with $2N-1$, $2N$, and $2N+1$ electrons, respectively. Let $\{t_i^-\}$, $\{t_i\}$, and $\{t_i^+\}$ be configurations which attain these minima. Let T^-, T, and T^+ be the associated T's and λ_i^-, λ_i, and λ_i^+ their eigenvalues. Then

$$\mu(2N+1)-\mu(2N)=\Delta^+ +\Delta^- +\lambda_{N+1}^+ -\lambda_N^-, \quad (13)$$

where

$$\Delta^{\pm} \overbrace{U(\{t_i^{\pm}\})}^{=} + 2\sum_1^N \lambda_i^{\pm} - U(\{t_i\}) - 2\sum_1^N \lambda_i. \quad (14)$$

The energy E for $2N$ electrons with the atoms in configuration $\{t_i^+\}$ is at least as large as the energy for $2N$ electrons with the atoms in configuration $\{t_i\}$, so that Δ^+ is nonnegative. The same reasoning shows that Δ^- is also nonnegative. Recall that T is unitarily equivalent to $-T$. This implies that the spectrum of T is symmetric about 0. Hence, $\lambda_{N+1}^+ \geq 0$ and $\lambda_N^- \leq 0$. Thus, Eq. (13) implies that $\mu(2N+1)-\mu(2N) \geq \Delta^+ + \lambda_{N+1}^+$.

We now consider three cases: (i)

$$\|(T^+)^2-T^2\| \leq (\lambda_{N+1})^2/2,$$

(ii)

$$\|(T^+)^2-\langle (T^+)^2\rangle\| \geq (\lambda_{N+1})^2/4,$$

and (iii)

$$\|\langle (T^+)^2\rangle \overbrace{T^2}^{-}\| \geq (\lambda_{N+1})^2/4.$$

By the triangle inequality, at least one of these cases must hold. We claim that λ_{N+1} is bounded away from zero, uniformly in N, for the following reason. When N is even or when N is odd and $N \geq$ some N_0, we have $\delta > 0$. Also, δ does not go to zero as $N \to \infty$. This implies the claim in the two cases just cited. If N is odd and $N < N_0$ then $\lambda_{N+1} > 0$ since 0 is not an eigenvalue of T in this case, even if $\delta=0$. (It is precisely for this reason that δ can be zero in the odd-N case.) Since N_0

is finite, this implies a positive lower bound to λ_{N+1} when $N < N_0$, which proves the claim.

In case (i), note that $(\lambda_{N+1})^2$ and $(\lambda^+_{N+1})^2$ are the smallest eigenvalues of T^2 and $(T^+)^2$. Then,

$$(T^+)^2 = T^2 + [(T^+)^2 - T^2] \geq T^2 - \|(T^+)^2 - T^2\|$$
$$\geq T^2 - (\lambda_{N+1})^2/2 \geq (\lambda_{N+1})^2/2,$$

and thus $(\lambda^+_{N+1})^2 \geq (\lambda_{N+1})^2/2$ which implies there is a gap. In case (ii) we bound Δ^+ as before except that we use the lemma in place of (6). This yields

$$\Delta^+ \geq \|T^+\|^{-3} \mathrm{Tr}[(T^+)^2 - \langle (T^+)^2 \rangle]^2. \quad (15)$$

Combining this with (ii), and the fact that $\mathrm{Tr}A^2 \geq \|A\|^2$ for Hermitean A, shows that Δ^+ is bounded away from zero. (The norm of T^+ is easily bounded from above.)

To handle case (iii) consider the dimerized configuration with the same y and x as $\langle (T^+)^2 \rangle$. Call these parameters y^+, x^+ [and $z^+ = 2(x^+)^2 - (y^+)^2$]. Since $\|\Omega\| \leq 2$, the triangle inequality and (iii) imply $|y^2 - (y^+)^2| + |z - z^+| \geq (\lambda_{N+1})^2/8$. Since λ_{N+1} is bounded away from zero, at least one of $|y - y^+|$ and $|x - x^+|$ must be bounded away from zero. A simple calculation using (9) then shows that $\Delta^+ = O(N)$, which more than suffices.

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Stability of the Peierls instability for ring-shaped molecules

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We investigate the conventional tight-binding model of L π electrons on a ring-shaped molecule of L atoms with nearest-neighbor hopping. The hopping amplitudes $t(w)$ depend on the atomic spacings w with an associated distortion energy $V(w)$. A Hubbard-type on-site interaction as well as nearest-neighbor repulsive potentials can also be included. We prove that when $L=4k+2$ the minimum energy E occurs either for equal spacing or for alternating spacings (dimerization); nothing more chaotic can occur. In particular, this statement is true for the Peierls-Hubbard Hamiltonian, which is the case of linear $t(w)$ and quadratic $V(w)$, i.e., $t(w)=t_0-\alpha w$ and $V(w)=k(w-a)^2$, but our results hold for any choice of couplings or functions $t(w)$ and $V(w)$. When $L=4k$ we prove that more chaotic minima *can* occur, as we show in an explicit example, but the alternating state is always asymptotically exact in the limit $L\to\infty$. Our analysis suggests three interesting conjectures about how dimerization stabilizes for large systems. We also treat the spin-Peierls problem and prove that nothing more chaotic than dimerization occurs for $L=4k+2$ *and* $L=4k$.

I. INTRODUCTION

To derive the shape (and other properties) of molecules from first principles has been an actively pursued goal since the early days of quantum mechanics. Many of the insights into the structure of molecules like benzene and its relatives have, however, been obtained using drastically simplified models. The Schrödinger equation for all the nuclei and electrons in such a molecule involves many dozens or even hundreds of degrees of freedom and, therefore, simpler models with a reduced number of degrees of freedom are a necessity. In the case of benzene the introduction of the Hückel model[1] played an important role. This model is standard textbook material for organic chemistry students (see, e.g., Ref. 2). London[3] used the Hückel model to explain the large diamagnetic anisotropy of aromatic compounds and certain other materials quite successfully. A similar approach was used earlier by Jones in his work on bismuth and bismuth alloys.[4]

In this paper we are interested in ring-shaped molecules of the type $(CH)_L$ for *even* L, the so-called *annulenes* (sometimes called cyclic polyenes). The Hückel model for $[L]$-annulene describes the L π electrons (one for each carbon atom) as hopping from one carbon atom to the next (tight-binding approximation). The carbon atoms are located at the L sites of a ring-shaped geometry, so $L+1\equiv 1$. The Coulomb interaction between the electrons is ignored in the Hückel model but we will include the Hubbard[5] on-site interaction, as in the work of Pariser and Parr[6] and Pople,[7] in our study (a nearest-neighbor repulsion can also be included)

$$H=-\sum_{j=1}^{L}\sum_{\sigma=\uparrow,\downarrow} t_j c_{j+1,\sigma}^{\dagger}c_{j\sigma}+\text{H.c.}$$
$$+U\sum_{j=1}^{L}(n_{j\uparrow}-\tfrac{1}{2})(n_{j\downarrow}-\tfrac{1}{2})\,. \qquad (1.1)$$

Here $c_{j+1,\sigma}^{\dagger}$ and $c_{j\sigma}$ are the usual fermion creation and annihilation operators for a particle of spin σ at site j. The number operators are $n_{j\sigma}=c_{j\sigma}^{\dagger}c_{j\sigma}$. The hopping matrix elements are real, but they can be multiplied by complex phases if a magnetic field is present. [In (1.1) we write $(n_{j\sigma}-\frac{1}{2})$ instead of the customary $n_{j\sigma}$; the difference amounts only to the addition of trivial terms in the Hamiltonian, but these are convenient because they ensure—via hole-particle symmetry—that the expected particle number in the grand-canonical ensemble is $\langle N\rangle=L$, i.e., the "half-filled band."] The real parameter U represents the strength of the on-site interaction of two particles and the Hückel approximation consists in setting $U=0$. The set of t_j's will be denoted by $\{t_j\}$. The dependence of the Hamiltonian on the parameters will be made explicit, where needed, with a notation of the type $H(\{t_j\})$, $H(\{t_j\},U)$, etc. For a review of rigorous results on the Hubbard model see Ref. 8.

The hopping matrix element t_j is a resonance integral between orbitals at the sites j and $j+1$ and therefore depends on the real space distance w_j between these sites. A typical choice is $t_j=t_0-\alpha w_j$.[9] A more realistic choice would be $t_j=t_0\exp(-\alpha w_j)$ or some other rapidly decaying function of w_j. If one adds to the Hubbard Hamiltonian (even in the Hückel approximation) a term describing the interaction between the carbon ions (the energy of lattice distortions) one obtains a model that, in spite of its extreme simplicity, serves very well to explain a number of phenomena in annulenes and linear $(CH)_x$ (polyacetylene).[10] For a recent review see Refs. 11 and 12. Although in more refined models the lattice distortions should be treated as quantum-mechanical phonons,[9] a more common choice, which we will follow here, is to describe them in the Born-Oppenheimer approximation by adding to the Hamiltonian (1.1) a classical potential of the form

$$\sum_{j=1}^{L} V(w_j)$$

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and to minimize, with respect to the w_j, the energy functional

$$\lambda_0(H(\{t(w_j)\}))+\sum_{j=1}^{L} V(w_j)\ ,$$

where $\lambda_0(H)$ denotes the lowest eigenvalue of H. Often V is taken to be quadratic, but in this paper we will *not* assume that V is quadratic or that the dependence of the t_j on the w_j is linear.

The Peierls instability[13] (discovered also by Fröhlich[14] and seemingly independently by Longuet-Higgins and Salem[15]) states that for L sufficiently large and U not too large, the minimum will not be attained in a translation invariant configuration of w_j's. By a straightforward computation (exact in the case $U=0$ or perturbative for small nonzero U) one can show that, for any fixed choice of the function V, there is an L_0 such that for all $L \geq L_0$ the ground-state energy of H with

$$w_j = w_0 + (-1)^j\delta\ , \tag{1.2}$$

for small δ, is lower than with the best choice of $w_j=$const. In the context of $(CH)_x$ molecules this was discovered independently by Labhart[16] and Ooshika.[17]

The phenomenon described by (1.2) is called *dimerization* in the physics literature. Unfortunately, this word has quite different connotations in the chemistry literature, but there does not seem to be a universally accepted terminology for (1.2) among chemists. The phrase *bond alternation*[15] would be a more accurate description as far as chemists are concerned. We are obliged to make a choice here, and we shall use "dimerization"—in the hope that chemists will substitute "bond alternation" for it in their minds. In fact, we shall go further and *declare a configuration to be dimerized, even if (1.2) holds with* $\delta=0$, i.e., the w_j's are translation invariant. In other words, a dimerized configuration is one with period-2 translation invariance, and this includes period 1 as a special case. This convention, while a bit unusual, conveniently eliminates awkward locutions.

For the Hückel model ($U=0$) and for $L=2$ mod4 (i.e., $L=6,10,14,\ldots$) the dimerization instability was shown very explicitly by Longuet-Higgins and Salem, who also estimated the degree of dimerization δ for realistic values of the parameters.[15] The physical mechanism for the occurrence of lattice distortions is rather simple and quite universal for electron-lattice systems in one dimension. A lattice distortion of period $1/2k_F$ opens up a gap at the Fermi level, thus lowering the energy of the occupied levels. This was a basic ingredient in Fröhlich's theory of superconductivity. The calculations mentioned above show that for small distortions this lowering of the energy exceeds the positive contribution to the total energy of the lattice distortion itself. In the infinite volume limit the elastic energy per bond is quadratic in the parameter δ of (1.2), while the electronic energy per bond decreases by an amount proportional to $\delta^2\ln\delta$ for small δ. As far as we know the first author who mentions this logarithmic behavior is Fröhlich in Ref. 14.

A common feature of the works mentioned above is that they always show that certain instabilities exist. The question of the "stability of the instabilities" is usually not raised, much less resolved. The main purpose of this work is to study the stability and instability of lattice distortions and to obtain rigorous statements about the *true* energy minimizing state. Longuet-Higgins and Salem[15] raised the question of the possible occurrence of higher periodicities but expected them to be unimportant. We prove that in the case $L=2$ mod4 (an assumption they made for technical reasons) they were right: *indeed nothing else than periodicity 2 occurs for* $L=2$ *mod4, but when* $L=0$ *mod4 other instabilities may, in fact, occur.*

For the Hückel model with $t=t_0-\alpha w$ and $V(w)=k(w-a)^2$, Kennedy and Lieb[18] showed that the true minimizing configuration is *always* of periodicity 2, i.e., w_j is of the form (1.2). Moreover, the minimizing configuration is unique (up to translations). It is remarkable that this result holds for *all even L*, in contrast with what will be proved here for general functions V.

We note parenthetically that the models we study are also used to describe electrons in mesoscopic metallic rings.[19] These rings are typically two orders of magnitude larger than the largest annulenes produced in the laboratory so far, and therefore the magnetic fields needed to obtain a flux through the ring of the order of a flux quantum are much smaller and experimentally accessible. The main issue is to calculate the persistent currents in such a ring threaded by a magnetic flux. Depending on the electron number, among other things, these currents can be paramagnetic or diamagnetic. Although most authors assume uniform hoppings t for this problem, there is an intimate connection between these persistent currents and the stability of dimerized configurations of t's.

In order to proceed to a precise formulation of our results it is first necessary to confront some possibly confusing questions about the phases of the t_j's. Let us write

$$t_j = |t_j|\exp[i\theta_j]\ ,$$

with $-\pi<\theta_j\leq\pi$. We note, first, that by a simple unitary gauge transformation of the type $c_{j\sigma}\to\exp[i\varphi_j]c_{j\sigma}$ and $c^\dagger_{j\sigma}\to\exp[-i\varphi_j]c^\dagger_{j\sigma}$, the operators $n_{j\sigma}$ and the energy levels of H are unchanged, but the t_j's change to $t_j\to t_j\exp[i(\varphi_j-\varphi_{j+1})]$. Consequently, the energy levels depend *only* on the "total flux" Φ of the t_j's defined by

$$\Phi=\arg\left[\prod_{j=1}^{L} t_j\right]\ ,$$

with $-\pi<\Phi\leq\pi$.

The next consideration comes from the physics of our model. The t_j's are real, unless there is a superimposed magnetic field, in the absence of which each $\theta_j=0$ or π, depending on whether t_j is positive or negative. Both signs can occur. Furthermore, it is understood that the t_j's remain close to some nonzero value in the physically realistic situation. Without loss of generality we can choose this value to be positive. With this in mind, we shall assume that the elastic energy, as a function of t, defined by

$$f(|t|)\equiv\inf\{V(w)|t(w)=t\}\ ,$$

depends only on $|t|$ and not on the sign of t. [We will impose below in (1.6) some other very mild physical conditions on f.] This is not to say that negative t's will not be permitted. They will—as we explain next.

Our procedure will be to study the total energy

$$\mathcal{E}_L(\{t_j\})\equiv\lambda_0(H(\{t_j\}))+\sum_{j=1}^{L}f(|t_j|)\ , \tag{1.3}$$

and to evaluate its minimum

$$E_L\equiv\min_{\{t_j\}}\mathcal{E}_L(\{t_j\})\ , \tag{1.4}$$

where the minimum is taken over all choices of $\{|t_j|\}$ *as well as* the phases $\{\theta_j\}$. Thus we allow negative t_j's and give them the same elastic energy as $|t_j|$. Since the t_j's are not expected to pass through zero in the physical case, this is no real restriction. In terms of the t_j, dimerization means that the configurations minimizing $\mathcal{E}_L(\{t_j\})$ are of the form

$$t_j=t_0+(-1)^j\delta\ . \tag{1.5}$$

It will turn out that for all L our theorems show that the energy minimizing t_j's are real (modulo a gauge transformation). But for $L=0\,\mathrm{mod}4$ an odd number of them *must* be negative for an energy minimizer—thereby precluding a dimerized state. If, on the other hand, we wish to attribute the occurrence of an odd number of negative t_j's to the presence of an external magnetic field then we can say that a dimerized state minimizes the energy in the presence of a field of flux π. Given that no such field is really present, we will have to conclude that the energy minimum will not be a dimerized state when $L=0\,\mathrm{mod}4$. In this case we can redefine our problem by restricting the minimum in (1.4) to positive t_j's. Do we get a dimerized state then? We do not know the general answer but we have some conjectures about this question. If $f(t)=k(t-a)^2$, as in Ref. 18, we know that a dimerized state is, indeed, the minimum.

The physical conditions we impose on f are

$$\begin{aligned}&\text{(i) } f \text{ is continuous ,}\\ &\text{(ii) } f(t)\geq Ct\end{aligned} \tag{1.6}$$

for large t and for some constant $C>4$.

The continuity of f is not really necessary for the validity of our results. In fact in the Appendix (Lemma 13) we show that f can always be replaced with a convex (and hence continuous) function without changing the minimizing configurations. Property (ii) is necessary to have a stable minimum at all, e.g., to prevent the molecule from collapsing to a point.

We minimize the ground-state energy $\mathcal{E}_L$ not only with respect to the parameters t_j but *also* with respect to the number of electrons. In Sec. II we prove that if $U\neq0$ and all t_j are real, the ground states of (1.1) will in fact necessarily have $N=L$. In this case all results below are equally valid for minimization of the energy with the particle number fixed at half filling. The condition $U\neq0$ is necessary in the case of rings of size $L=0\,\mathrm{mod}4$, for with $U=0$ the model with translation invariant t's has ground states with particle number ranging from $L-2$ to $L+2$, due to zero eigenvalues of the one-particle Hamiltonian.

A. Relation with the flux-phase problem

The minimization with respect to the flux Φ of $\mathcal{E}_L(\{t_j\})$, for fixed $|t_j|$, is a generalization of the so-called flux-phase problem[20,21] for rings. In the case $U=0$ (as in the original formulation of this problem), but arbitrary, *fixed*, positive $\{t_j\}$, this problem was solved by Lieb and Loss.[22] The arguments of this paper provide a way of solving the problem for rings and all values of U (Corollary 8). For rings of length $L=2\,\mathrm{mod}4$ the optimal (that is, energy minimizing) flux is 0. When $L=0\,\mathrm{mod}4$, the optimal flux is $\Phi=\pi$. This can be extended to higher dimensions[23] when some geometric periodicity is present. In particular, Ref. 23 proves the conjecture that the optimal flux for the Hubbard model on the two-dimensional square lattice is π through each plaquette.

B. Main results

The following theorem, which we prove in Sec. III, says that, when $L=2\,\mathrm{mod}4$ and the flux is zero and when $L=0\,\mathrm{mod}4$ and the flux is π, the Peierls instability is itself stable in the sense that no other lattice distortions than period 2 can occur. The theorem does *not* state that distortion always happens. Depending on the parameters in the Hamiltonian, the function f in particular, the energy minimizing configuration may or may not be translation invariant. In real molecules both situations occur. Benzene, e.g., has all C-C bond lengths equal (within the precision of today's measurements and in agreement with the analysis of Labhart[16] and Ooshika[24]), while for large rings or long chains the Peierls instability will necessarily lead to two different bond lengths.

Theorem 1 (minimizing configurations). (i) If $L=2\,\mathrm{mod}4$, the minimum of $\mathcal{E}_L$ is attained in a dimerized configuration of the form (1.5) in which the t_j's are all positive (or all negative). (ii) If $L=0\,\mathrm{mod}4$, the minimum of $\mathcal{E}_L$ is attained in a configuration in which the $|t_j|$'s satisfy (1.5) but the flux Φ equals π.

That the cases $L=2\,\mathrm{mod}4$ and $0\,\mathrm{mod}4$ behave differently with respect to the flux was noted a long time ago (see, e.g., the "Hückel rule" in Ref. 2). The $U=0$ one-electron problem has zero-energy states when $L=0\,\mathrm{mod}4$ but not when $L=2\,\mathrm{mod}4$. In the first case this leads to diamagnetic, in the second case to paramagnetic response to magnetic fields, as was noted in Ref. 3 and as is observed experimentally in the annulenes.[25]

Theorem 2 (uniqueness). If there is only one (up to translation and gauge transformations) dimerized configuration satisfying the conclusion of Theorem 1, then there are no other energy minimizing configurations.

We define three additional minimization problems for the $L=0\,\mathrm{mod}4$ case.

(1) Zero-flux problem. We restrict the minimization in (1.4) to those $\{t_j\}$ with zero flux, i.e., $\Phi=0$.

(2) Period-2 problem. In addition to $\Phi=0$ we make the

further restriction that the t_j's must be dimerized.

(3) The infinite-chain problem. Let $d(x,y)$ denote the dimerized configuration with $t_{2j+1}=x$ and $t_{2j}=y$, and minimize the energy per site defined by

$$e(x,y)=\lim_{L\to\infty}\frac{1}{L}\mathcal{E}_L(d(x,y))\,. \tag{1.7}$$

The minimum energy in the first case is denoted by E_L^0, and the t_j's by t_j^0. The second energy is denoted by $E_{L,\text{dimer}}^0$ and the t_j's by $t_{j,\text{dimer}}^0$. Clearly

$$E_{L,\text{dimer}}^0 \geq E_L^0$$

and one of our conjectures below concerns the case of equality. The following, however, shows that the three problems become asymptotically the same (to within two powers of L^{-1}, instead of merely one) as $L\to\infty$.

Theorem 3 (asymptotic dimerization). (i) Assume that there is a unique energy minimizing dimerized configuration $d(x,y), x\geq y$, for the infinite-chain problem. Then any sequence of minimizing configurations $\{t_j^0\}$ of the zero-flux problem converges to a dimerized configuration as $L\to\infty$. Namely,

$$\lim_{L\to\infty}\max_j |t_j^0-t_{j,\text{dimer}}^0|=\lim_{L\to\infty}\max_j |t_j^0-d(x,y)_j|=0\,,$$

where we have adopted the convention that t_1 is the largest of the t_j's for all configurations. (ii) For any even L, the energies satisfy

$$0\leq E_{L,\text{dimer}}-E_L^0\leq \text{const}\times L^{-1}\,.$$

In Sec. V we discuss the situation of finite rings of length $L=0\,\text{mod}4$. Instabilities other than period 2 can exist for arbitrarily large rings if the function f is chosen appropriately. An optimally dimerized ring of size $L=0\,\text{mod}4$ can have other instabilities and it seems that the strongest of those actually has wavelength equal to L, and is not, as one could have expected, of period 4 or some other higher periodicity. We illustrate this with an explicit example of a ring of eight sites for which the minimum is not period 2. A perturbative analysis indicates that the conditions on f for a further instability to occur become more stringent as the system becomes larger. In particular, the dimerization itself has to be smaller as L becomes bigger. This leads us to the following two conjectures.

Conjecture 1. For every $L=0\,\text{mod}4$ there exists a function f (depending on L), satisfying conditions (i) and (ii) in (1.6), such that the energy minimizing configurations for the zero-flux problem are *not* period 2.

Conjecture 2. For any fixed f satisfying (1.6), and such that there is a unique minimum for the infinite-chain problem, there is a critical size L_c such that for all even $L\geq L_c$ all zero-flux minima are period 2.

C. The spin-Peierls problem

Another closely related question is the spin-Peierls problem. For U large and positive, and half filling, the Hubbard model reduces to the Heisenberg antiferromagnetic spin chain in second-order perturbation theory.[26] The spin chain also has an instability when coupled to lattice distortions, as was pointed out by Chesnut[27] and by Beni and Pincus.[28,29] More explicitly one looks for the configurations of coupling constants J_{ij} that minimize the smallest eigenvalue of the Hamiltonian:

$$H_\Lambda=\sum_{\langle i,j\rangle}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j+\sum_{\langle i,j\rangle}f(J_{ij})\,, \tag{1.8}$$

where the sum is over nearest-neighbor pairs in a finite subset Λ of the hypercubic lattice, and $f(J_{ij})$ is the elastic energy as before. In one dimension Cross and Fisher[30] computed the exponent governing the ground-state energy density $e(\delta)$ of the system with alternating couplings:

$$J_j=1+(-1)^j\delta\,,$$

with $J_j\equiv J_{j,j+1}$. They found that, up to logarithmic corrections,

$$|e(\delta)-e(0)|\sim-|\delta|^{4/3}\,.$$

Numerical confirmation of this exponent and evidence for a logarithmic correction was reported in Ref. 31. The important point here is that $\frac{4}{3}<2$, which implies the instability of the translation invariant configurations under period-2 perturbations, provided f has a finite second derivative. It was recently proved that this exponent is identical to a critical exponent of the two-dimensional four-state Potts model.[32]

The question addressed in this paper is again to determine the nature of the minimizing configurations. It turns out that the true minimum is dimerized for *any* (even) system size and in *any* dimension. *The 2 mod4 versus 0 mod4 dichotomy does not arise for the Heisenberg model.*

Theorem 4 (dimerization for spin Peierls). Let $\Lambda\subset\mathbb{Z}^d$ be a rectangular box of even size in all coordinate directions and with periodic boundary conditions. Then there is an energy minimizing configuration of J_{ij}'s which is of periodicity 2 in all coordinate directions.

This theorem prompts one more conjecture.

Conjecture 3. Suppose that a minimizer for the zero-flux problem for some f and $L=0\,\text{mod}4$ and some $U_0\geq 0$ is a dimerized state. Then for every $U>U_0$ there is a dimerized minimizer for the zero-flux problem with the same f and L. In particular, the truth of this conjecture, when combined with the $U=0$ result in Ref. 18, would imply that, with a quadratic f, dimerization always occurs, even in the $L=0\,\text{mod}4$ case.

D. Extensions of the results presented in this paper

(1) It has been argued that the Hubbard on-site repulsion does not describe the Coulomb interaction between the electrons accurately enough (for a discussion see, e.g., the reviews on this topic in Ref. 33, and references therein). While the Hubbard term alone, when not too large, seems to have the effect of enhancing the dimerization,[34] taking into account some nearest-neighbor interaction terms Kivelson, Su, Schriefer, and Heeger[35] found that the Coulomb repulsion in fact suppresses the dimerization in polyacetylene. Without entering into this dis-

cussion here we would like to point out that without substantial modification one can prove the results of Theorems 1 and 2 for a Hamiltonian that includes a repulsive nearest-neighbor interaction of the form

$$\sum_j W(t_j)(n_j-1)(n_{j+1}-1) .$$

The -1's are inserted to keep the chemical potential tuned at half filling. We require $W(t)\geq 0$, but no assumption on the dependence of W on t is needed. Theorem 1 holds unchanged, but we can extend the proof that the grand-canonical ground states are necessarily half filled only under the additional condition that $W(t_{j-1})+W(t_j)<U_j$, for all t's in the relevant range. Nearest-neighbor exchange terms and certain longer-range interactions can also be treated.

(2) Instead of a homogeneous on-site repulsion it is sometimes more realistic to have different U for different (classes of) sites, e.g., in a periodic manner. Theorem 1 extends to such situations in the following sense: The minimum energy will be attained in a configuration of t_j which is invariant under all reflections through planes that intersect two opposite bonds on the ring (as indicated by a dashed line in Fig. 1) and that leave the configuration of the U_i invariant. As an example consider [18]-annulene. Of the 18 hydrogens in this molecule 6 reside inside the ring and 12 outside, according to the pattern: 1 inside, 2 outside, 1 inside, etc. A possible way of taking the effect of this periodic configurations of H atoms into account is to add a periodic one-particle potential to the Hamiltonian. In the present example this potential would take two different values and depend on the site according to the pattern $(v_i)=(v_1,v_1,v_2,v_1,v_1,\ldots)$. Our general result then implies an energy minimizing configuration of C-C bonds of the form $ABCACBABCACB\ldots$. The observed bond lengths in [18]-annulene indeed satisfy this pattern [they are $A=1.419$ Å, $B=1.382$ Å, $C=B$ (Ref. 25)].

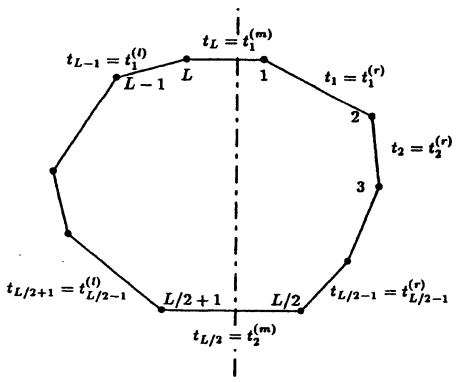

FIG. 1. A ring containing an even number of sites, labeled $1,\ldots,L$. The hopping matrix element t_j is associated with the bond $\{j,j+1\}$. Reflection through the plane indicated by the dashed line interchanges the role of the hoppings labeled $t^{(l)}$ and the ones labeled $t^{(r)}$ (see Lemma 7).

(3) Hubbard models with spin-dependent hoppings, i.e., $t_j=|t_j|m_j,m_j\in SU(2)$, have been considered in the literature in order to study the effects of spin-orbit coupling.[36-38] By virtue of the SU(2) gauge symmetry of the Hamiltonian one can diagonalize the spin dependence of the hoppings up to an SU(2) flux, which is defined up to an SU(2) transformation by the matrix $M=m_1m_2m_3\cdots m_L$. The methods of this paper can be used to prove the existence of a minimizer having dimerization and $M=1$ when $L=2\,\mathrm{mod}4$ and when $L=0\,\mathrm{mod}4$ a minimizer has $M=-1$ and dimerization. This is completely analogous to the U(1) case treated in Theorem 1.

(4) Mattis and Langer[39] introduced a simple model to study the interaction between the electrons and a phonon instability of the Peierls type as a function of the temperature. Our methods can also be used to prove that in this model the electron state has periodicity 2 and that its correlations indicate dimerization. For a rigorous study of the Kohn anomaly, which accompanies the phase transition in the Mattis-Langer model, see Ref. 40.

Generalizations that are not considered in this work include the interaction between the electrons and lattice in excited states, the effects of doping, and higher-dimensional models. Low-lying electronic excited states can induce further (e.g., solitonlike) distortions of the lattice.[9,41,42] In doped polyacetylene an interesting semiconductor-metal transition occurs.[43] Away from half filling, instabilities other than period-2 will naturally develop (see, e.g., Ref. 44, and references therein). In two dimensions, e.g., on a square lattice, $2k_F$ instabilities may develop either in the coordinate directions or in the diagonal directions.[45,46] This may be related to the non-period-2 instabilities that can occur in rings whose size is a multiple of 4, e.g., in the elementary plaquettes of the square lattice. Another new feature of higher dimensions is that the breaking of translation invariance can occur at nonzero temperature. This has been rigorously shown to occur in the Falicov-Kimball model[47,48] and in the Holstein model.[49]

II. THE GRAND-CANONICAL HUBBARD MODEL AT HALF FILLING

In the definition of the energy functional (1.3) we used the lowest eigenvalue of the grand-canonical Hubbard Hamiltonian at half filling. Our goal in this section is to prove that the corresponding ground state necessarily has $N=L$ if we assume the t_j's are real (as will later be shown to be the case). It is then obvious that minimization of the energy with respect to the parameters t_j *and* the number of electrons produces exactly the same minimizing configurations as the restricted minimization with the particle number fixed at $N=L$. The arguments in this section are not restricted to one dimension. We believe they are interesting in their own right and can be of interest in a more general context. Therefore we temporarily consider a more general setup on a general finite

lattice Λ, the number of whose lattice sites is denoted by $|\Lambda|$.

Consider the grand-canonical Hubbard Hamiltonian (1.1) for spin-$\frac{1}{2}$ fermions on Λ, and with arbitrary chemical potential μ:

$$H_\mu = -\sum_{i,j\in\Lambda}\sum_{\sigma=\uparrow,\downarrow} t_{ij}c_{j\sigma}^\dagger c_{i\sigma} + \sum_{j\in\Lambda} U_j(n_{j\uparrow}-\mu)(n_{j\downarrow}-\mu) .$$

The t_{ij} are assumed (in this section only) to be real and symmetric, i.e., $t_{ij}=t_{ji}$. Λ is assumed to be connected, i.e., given i and j in Λ we can find a sequence $i=i_1,i_2,\ldots,i_m=j$ such that $t_{i_1,i_2}t_{i_2,i_3}\cdots t_{i_{m-1},i_m}\neq 0$. The U_j and μ are also real parameters. As before the dependence of H on its parameters will be made explicit with a notation of the type H_μ, $H(\{t_{ij}\})$, $H_\mu(\{t_{ij}\},\{U_j\})$, etc. When H appears without subscript the chemical potential is $\mu=\frac{1}{2}$, corresponding to half filling.

The spin-up and spin-down particle number operators are defined by

$$N_\sigma = \sum_{j\in\Lambda} n_{j\sigma} ,$$

where $\sigma=\uparrow,\downarrow$ and $n_{j\sigma}=c_{j\sigma}^\dagger c_{j\sigma}$. Note that $N_\uparrow$ and $N_\downarrow$ each commute with H, and hence their eigenvalues are good quantum numbers. H also commutes with the total-spin operators (which generate the global spin rotations) given by

$$S^+=\sum_j c_{j\uparrow}^\dagger c_{j\downarrow},\quad S^-=\sum_j c_{j\downarrow}^\dagger c_{j\uparrow},\quad S^3=\tfrac{1}{2}(N_\uparrow-N_\downarrow) .$$

Therefore, by applying S^+ or S^- an appropriate number of times, one can transform any ground state of H into a ground state with

$$N_\uparrow - N_\downarrow = \begin{cases} 0 & \text{if } N \text{ is even} \\ \pm 1 & \text{if } N \text{ is odd} . \end{cases} \tag{2.1}$$

We say that Λ and t are bipartite if the sites of Λ can be written as the disjoint union of two subsets; i.e., $\Lambda=\Lambda_A\cup\Lambda_B$, in such a way that the matrix t of hopping matrix elements respects this structure, namely, $t_{ij}=0$ if $i\in\Lambda_A$ and $j\in\Lambda_A$ or if $i\in\Lambda_B$ and $j\in\Lambda_B$. In this case the Hamiltonians $H_{1/2}(\{t_{ij}\},\{U_j\})$ and $H_{1/2}(\{t_{ij}\},\{-U_j\})$ are unitarily equivalent, i.e., at half filling ($\mu=\frac{1}{2}$) a global sign change of the potential does not affect the spectrum. A unitary transformation implementing this equivalence is the particle-hole transformation mapping

$$c_{j\uparrow}^\dagger \to \varepsilon(j)c_{j\uparrow},\quad c_{j\uparrow}\to\varepsilon(j)c_{j\uparrow}^\dagger ,$$
$$c_{j\downarrow}^\dagger \to c_{j\downarrow}^\dagger,\quad c_{j\downarrow}\to c_{j\downarrow} ,$$

where $\varepsilon(j)=1$ for $j\in\Lambda_A$ and $\varepsilon(j)=-1$ for $j\in\Lambda_B$. By the same transformation the spin operators are mapped into the so-called *pseudospin* operators defined by

$$\bar S^+=\sum_j \varepsilon(j)c_{j\uparrow}c_{j\downarrow},\quad \bar S^-=\sum_j \varepsilon(j)c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger ,$$
$$\bar S^3=\tfrac{1}{2}(|\Lambda|-N_\uparrow-N_\downarrow) .$$

These operators therefore also commute with the Hamiltonian, and they also commute with the spin operators and generate an additional SU(2) symmetry. Under the particle-hole transformation $N_\uparrow$ and $N_\downarrow$ are transformed into $|\Lambda|-N_\uparrow$ and $N_\downarrow$, respectively. It is then obvious that by applying $\bar S^\pm$ to any ground state we can obtain a ground state with

$$N_\uparrow+N_\downarrow = \begin{cases} |\Lambda| & \text{if } N-|\Lambda| \text{ is even} \\ |\Lambda|\pm 1 & \text{if } N-|\Lambda| \text{ is odd} . \end{cases} \tag{2.2}$$

As the spin and pseudospin operators commute (2.1) and (2.2) can be realized simultaneously. For an even bipartite lattice and $\mu=\frac{1}{2}$ this implies that there is a ground state of H with $N_\uparrow=N_\downarrow=|\Lambda|/2$ or $N_\uparrow=N_\downarrow\pm 1=|\Lambda|/2$.

From the next lemma it will follow that if in addition all U_j are nonvanishing and of the same sign, *all* ground states have even particle number and satisfy $N_\uparrow=N_\downarrow=|\Lambda|/2$. Note that the lemma itself does not require Λ to be bipartite.

Lemma 5. If all t_{ij} are real and $U_j\le 0$ for all j, then the ground-state space of $H(\{t_{ij}\},\{U_j\})$ contains a state with $N_\uparrow=N_\downarrow$. If $U_j<0$ for all j, all ground states satisfy $N_\uparrow=N_\downarrow$. In particular, the total number of particles in the ground state is even and the total spin is zero.

Proof. We can introduce new operators $\hat c_{i,\sigma}$ defined by

$$\hat c_{j,\uparrow}=c_{j,\uparrow},\quad \hat c_{j,\downarrow}=(-1)^{N_\uparrow}c_{j,\downarrow} .$$

H has then the same form in terms of the $\hat c$'s as in terms of the c's, but now the $\hat c_{j,\downarrow}^\#$ commute with the $\hat c_{j,\uparrow}^\#$.

Our Hamiltonian is now an operator on $\mathcal{H}_\uparrow\otimes\mathcal{H}_\downarrow$, and can be written in the form

$$H = T\otimes 1 + 1\otimes T + \sum_{i\in\Lambda} U_j(n_j-\mu)\otimes(n_j-\mu) ,$$

where $T=-\sum_{i,j\in\Lambda}t_{ij}c_j^\dagger c_i$. (Because spin-up and spin-down operators act identically on different tensor factors in the Hilbert space, we can omit the spin index.) T and the n_j are real in the canonical basis of localized particles. Therefore we can apply Lemma 14 of the Appendix and the discussion thereafter to conclude that H has a ground state with $N_\uparrow=N_\downarrow$.

If $U_j<0$ for all i, there cannot be a ground state with $N_\uparrow\neq N_\downarrow$. Indeed the last statement of Lemma 14 implies that for any ground state Ω

$$U_j\langle\Omega|(n_{j,\uparrow}-\mu)\Omega\rangle = U_j\langle\Omega|(n_{j,\downarrow}-\mu)\Omega\rangle .$$

If $U_j<0$ this implies $N_\uparrow=N_\downarrow$. Q.E.D.

Lemma 6. If all t_{ij} are real and bipartite, $|\Lambda_A|=|\Lambda_B|$, and either all $U_j>0$ or all $U_j<0$, then the ground state of H with $\mu=\frac{1}{2}$ is unique and has $N_\uparrow=N_\downarrow=|\Lambda|/2$.

Proof. It is sufficient to consider the case of all $U_j>0$. The case $U_j<0$ then follows because the particle-hole transformation changes the sign of the U_j, and the properties $N_\uparrow=|\Lambda|/2$ and $N_\downarrow=|\Lambda|/2$ are unchanged under the transformation. Let us therefore consider the case $U_j>0$, for all j.

We first apply Lemma 5 to the particle-hole

transformed Hamiltonian which has all $U_j<0$. This tells us that $N_\downarrow=|\Lambda|-N_\uparrow$ in all ground states. In particular, the total number of particles is $|\Lambda|$ which, by assumption, is even. Then, by Theorem 2 of Ref. 50 (the grand-canonical version at half filling does not need the homogeneity of the potential) and the assumptions on the lattice, $N_\uparrow=N_\downarrow=|\Lambda|/2$. [Note: Theorem 2 of Ref. 50 requires $U_j=$const. That is the case when the interaction is $n_{j\uparrow}n_{j\downarrow}$ as in Ref. 50. If we use the formulation of (1.1), however, with $(n_{j\uparrow}-\frac{1}{2})(n_{j\downarrow}-\frac{1}{2})$, the same proof works without the need of constant U_j.] Q.E.D.

For translation invariant t_{ij} on regular lattices the case $U_j\equiv 0$ is of course exactly solvable. It is rather straightforward in such cases to determine the ground-state degeneracy "by hand." The ground state is unique if and only if the eigenvalues of the matrix (t_{ij}) are all nonzero.

It is straightforward to extend Lemma 5 to Hamiltonians that include interactions of the form

$$F(\{n_{j,\uparrow}\})+F(\{n_{j,\downarrow}\})-\sum_\alpha G_\alpha(\{n_{j,\uparrow}\})G_\alpha(\{n_{j,\downarrow}\})$$

for arbitrary real functions F and G of the local particle numbers. One can use this to prove a slightly weaker form of Lemma 6 for a class of models with an additional term of the form

$$-\sum_{ij} W_{ij}(n_i-1)(n_j-1)$$

added to the Hamiltonian H. For these models our methods also prove that (i) if $W_{ij}\geq 0$ and $(U_j-\sum_i W_{ij})\geq 0$, for all j, then there is a ground state with $N_\uparrow=N_\downarrow=|\Lambda|/2$, and .(ii) if $W_{ij}\geq 0$ and $(U_j-\sum_i W_{ij})>0$, all ground states have $N_\uparrow=N_\downarrow=|\Lambda|/2$.

III. GENERAL RESULTS BASED ON REFLECTION POSITIVITY; PROOFS OF THEOREMS 1 AND 4

We now return to the half-filled Hubbard model ($N=|\Lambda|$) on a ring of even length $|\Lambda|=L$. It will be convenient to express the dependence of the energy functional on $\{t_j\}$ in a more explicit way. We write

$$\mathcal{E}_L(t^{(l)},t^{(m)},t^{(r)})=\lambda_0(H(\{t_j\}))+\sum_{j=1}^{L} f(|t_j|)\,,$$

where $t^{(l)}$, $t^{(r)}$, and $t^{(m)}$ denote a partition of the *complex* t_j's (with t_j^* denoting the complex conjugate of t_j) into three groups as follows (also see Fig. 1):

$$t^{(r)}=(t_1,\ldots,t_{L/2-1}),\quad t^{(m)}=(t_L,t_{L/2})\,,$$
$$t^{(l)}=(t_{L-1},\ldots,t_{L/2+1})\,.$$

The reflection of a configuration $(t^{(l)},t^{(m)},t^{(r)})$ through the plane intersecting the bonds $\{L,1\}$ and $\{L/2,L/2+1\}$ is the configuration $(t^{(r)},t^{(m)},t^{(l)})$, i.e., with $t^{(l)}\leftrightarrow t^{(r)}$.

Throughout this section we assume a constant potential $U_j=U$. The following lemma can be formulated to include nonconstant potentials but this is not needed for our purposes.

Lemma 7. Assume a constant potential $U_j=U$. If $L=2\,mod4$, assume that $t_{L/2}$ and t_L are real and nonnegative. If $L=0\,mod4$, assume that $t_{L/2}\geq 0$ and $t_L\leq 0$. The other t_j are allowed to be arbitrary complex numbers. Then the energy functional satisfies

$$\mathcal{E}_L(t^{(l)},t^{(m)},t^{(r)})\geq\tfrac{1}{2}[\mathcal{E}_L(t^{(l)},t^{(m)},t^{(l)*})+\mathcal{E}_L(t^{(r)*},t^{(m)},t^{(r)})]\,. \tag{3.1}$$

Proof. As in the proof of Lemma 5 we consider the Hamiltonian (1.1) as acting on $\mathcal{H}_\uparrow\otimes\mathcal{H}_\downarrow$, which amounts to considering operators referring to opposite spins as commuting. For $\sigma=\uparrow,\downarrow$ define a set of "spin" operators using a Jordan-Wigner transformation as follows:

$$S^3_{j,\sigma}=c^\dagger_{j,\sigma}c_{j,\sigma}-\tfrac{1}{2},\quad \mathbf{S}_{j,\sigma}=2S^3_{j,\sigma}\,,$$
$$S^+_{j,\sigma}=\mathbf{S}_{1,\sigma}\cdots\mathbf{S}_{j-1,\sigma}c^\dagger_{j,\sigma},\quad S^-_{j,\sigma}=\mathbf{S}_{1,\sigma}\cdots\mathbf{S}_{j-1,\sigma}c_{j,\sigma}\,.$$

With these definitions and the anticommutation relations of the $c_{i,\sigma}$ and $c^\dagger_{i,\sigma}$ it is straightforward to check that $S^3_{i,\sigma}$, $S^+_{i,\sigma}$, and $S^-_{i,\sigma}$ satisfy the standard SU(2) commutation relations and that they commute for different indices i,σ. In terms of these operators, and using the commutation relations, the Hamiltonian can be written as

$$H=\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow} t_jS^+_{j+1,\sigma}S^-_{j,\sigma}+\text{H.c.}+U\sum_{j=1}^{L}S^3_{j,\uparrow}S^3_{j,\downarrow}+t_L\sum_{\sigma=\uparrow,\downarrow}S^+_{1,\sigma}(\mathbf{S}_{1,\sigma}\cdots\mathbf{S}_{L,\sigma})S^-_{L,\sigma}+\text{H.c.}$$

By performing a rotation by π about the 2-axis at every other site and for both $\sigma=\uparrow$ and $\sigma=\downarrow$ we find that this spin Hamiltonian is unitarily equivalent to

$$\tilde{H}=\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}-t_jS^+_{j+1,\sigma}S^+_{j,\sigma}+\text{H.c.}+\sum_{j=1}^{L}U_jS^3_{j,\uparrow}S^3_{j,\downarrow}+(-1)^{L/2}t_L\sum_{\sigma=\uparrow,\downarrow}S^+_{1,\sigma}(\mathbf{S}_{1,\sigma}\cdots\mathbf{S}_{L/2,\sigma})\times S^+_{L,\sigma}(\mathbf{S}_{L,\sigma}\cdots\mathbf{S}_{L/2+1,\sigma})+\text{H.c.}$$

Under the conditions stated in the proposition $t_{L/2}\geq 0$ and $(-1)^{L/2}t_L\leq 0$. We can now apply Lemma 14 of the Appendix to $\tilde{H}$ with

$$A=-\sum_{j=1}^{L/2-1}\sum_{\sigma=\uparrow,\downarrow}t_jS^+_{j+1,\sigma}S^+_{j,\sigma}+\text{H.c.}+U\sum_{j=1}^{L/2}S^3_{j,\uparrow}S^3_{j,\downarrow}\,,$$

$$B=-\sum_{j=L/2+1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}t_jS^+_{j+1,\sigma}S^+_{j,\sigma}+\text{H.c.}+U\sum_{j=L/2+1}^{L}S^3_{j\uparrow}S^3_{j\downarrow}\,,$$

$$C_1\otimes C_1=t_{L/2}S^+_{L/2+1,\uparrow}S^+_{L/2,\uparrow}\,,$$

$$C_2 \otimes C_2 = |t_L| S^+_{1,\uparrow}(S_{1,\uparrow} \cdots S_{L/2,\uparrow}) \times S^+_{L,\uparrow}(S_{L,\uparrow} \cdots S_{L/2+1,\uparrow}) ,$$

and six more terms $C_i \otimes C_i$, $i = 3, \ldots, 8$, which are equal to $C_1 \otimes C_1$ and $C_2 \otimes C_2$ with $\uparrow$ replaced by $\downarrow$ and the Hermitian conjugates of these operators. This gives us the inequality of the lemma for the lowest eigenvalue of H. The elastic energy terms in the functional $\mathcal{E}_L$ add up to the same contribution on both sides of the inequality and therefore can be included trivially. Q.E.D.

Proof of Theorem 1. First we prove that the minimum of $\mathcal{E}_L$ is attained in a configuration of t_j with total flux $\Phi = 0$ when $L = 2 \bmod 4$, and with $\Phi = \pi$ when $L = 0 \bmod 4$. Let $\{t_j\}$ be minimizing. Due to the invariance of the ground-state energy of H under gauge transformations, the energy functional $\mathcal{E}_L$ defined in (1.3) depends only on $\{|t_j|\}$ and Φ. Hence, for any set of t_j's, there are t'_j such that $\mathcal{E}_L(\{t_j\}) = \mathcal{E}_L(\{t'_j\})$ and $t'_{L/2}$ and t'_L are real and have the correct sign for application of Lemma 7. The two configurations in the right side of (3.1) have flux $\Phi = \arg(t'_{L/2} t'_L)$ which, by assumption, takes the values stated in the theorem. Because $\{t_j\}$ is minimizing, (3.1) must be an equality. Therefore the two configurations on the right side must be minimizers of $\mathcal{E}_L$, but then both have the correct flux, 0 or π.

Next we show that in both cases the minimum of $\mathcal{E}_L$ is attained in a configuration with $\{|t_j|\}$ dimerized. For any configuration $(t^{(l)}, t^{(m)}, t^{(r)})$ of real t_j's and $t^{(m)}$ of the right signs, (3.1) implies that either $(t^{(l)}, t^{(m)}, t^{(l)})$ or $(t^{(r)}, t^{(m)}, t^{(r)})$ has at least as low an energy and has at least as many pairs of identical $|t_j|$'s. In particular, this shows that $\mathcal{E}_L$ is minimized in a configuration with $|t_j| = |t_{j+2}|$ for $j = L/2 - 1$ and $j = L - 1$. Because $\mathcal{E}_L$ is translation invariant the argument above can be repeated to show that there is a minimizing configuration with $|t_j| = |t_{j+2}|$ for all j, which is the desired result. Q.E.D.

Lemma 7 also permits us to solve the flux-phase problem for even rings with $U \neq 0$.

Corollary 8. Let $U_j \equiv U$ and let $\{t_j\}$ be a fixed configuration of non-negative t_j's. Then the minimum of $\mathcal{E}_L$, varying over the total flux Φ alone, is attained for $\Phi = 0$ if $L = 2 \bmod 4$ and for $\Phi = \pi$ if $L = 0 \bmod 4$.

Proof of Theorem 4. The Heisenberg antiferromagnet on an arbitrary bipartite lattice is reflection positive.[51] This implies, via Lemma 14, the following inequality, analogous to Lemma 7:

$$\lambda_0(H_{\text{Heis}}(\{J^{(l)}_{ij}, J^{(m)}_{ij}, J^{(r)}_{ij}\})) \geq \tfrac{1}{2}[\lambda_0(H_{\text{Heis}}(\{J^{(l)}_{ij}, J^{(m)}_{ij}, J^{(l)}_{ij}\})) + \lambda_0(H_{\text{Heis}}(\{J^{(r)}_{ij}, J^{(m)}_{ij}, J^{(r)}_{ij}\}))] ,$$

where $\{J^{(l)}_{ij}, J^{(m)}_{ij}, J^{(r)}_{ij}\}$ denotes a partition of the coupling constants into three groups: the $J^{(l)}_{ij}$ are the couplings on the bonds to the left of any reflection plane of the lattice, the $J^{(m)}_{ij}$ are the couplings on the bonds intersected by the reflection plane, and the $J^{(r)}_{ij}$ are the coupling to the right of the plane. Using this inequality Theorem 4 is then proved in the same way as Theorem 1, but this time there is no need to distinguish between $L = 0 \bmod 4$ and $L = 2 \bmod 4$—or even to restrict ourselves to one dimension. Q.E.D.

IV. ASYMPTOTIC DIMERIZATION FOR $L = 0 \bmod 4$; PROOFS OF THEOREMS 2 AND 3

Even though finite rings of length $L = 0 \bmod 4$ can do more complicated things than dimerize (see Sec. V for a discussion of counterexamples), they do dimerize asymptotically. To be precise, for a fixed f, satisfying condition (i) and (ii) of (1.6), for which the infinite ring has a unique energy minimizing configuration among the configurations of period 2, any sequence of minimizers for finite rings has to approach that dimerized configuration uniformly when $L \to \infty$, i.e., any nearest pair of $|t_j|$'s converges to the pair occurring in the infinite volume dimerized configuration. The aim of this section is to prove this statement, which is Theorem 3(i). At the same time we will also supply the proofs of Theorems 2 and 3(ii).

In contrast to the preceding section, here we will always consider minimization of the energy over arbitrary configurations of $|t_j|$, but with constant flux Φ. For this purpose it is convenient to introduce an explicit notation for the energy functionals at fixed Φ:

$$\mathcal{E}^{\Phi}_L(\{t_j\}) = \mathcal{E}_L(\{e^{i\Phi/L} t_j\}) .$$

Here, and in the rest of this section, it is assumed that all t_j are non-negative. Note that the t_j's now play the role of the $|t_j|$'s.

For any x and y let $d(x,y)$ denote the configuration with $t_j = x$ for j odd and $t_j = y$ for j even, and define the energy density e of a period-2 configuration $d(x,y)$ as in (1.7). Note that e is independent of Φ. In order to remove the degeneracy due to the obvious symmetry under cyclic permutations of the t_j's, we will henceforth adopt the convention that the maximum value of all t's is attained by t_1.

A first ingredient in the proof of Theorem 3 is the following energy estimate, which by itself implies Theorem 3(ii). Let E^{Φ}_L denote the value of $\mathcal{E}^{\Phi}_L$ in a minimizing configuration $t^{\Phi}_{L,j}$. Under the general condition (1.6), (ii) on f we can find a constant K, depending only on f, such that $|t^{\Phi}_{L,j}| \leq K$.

Lemma 9. Assuming only condition (ii) on f in (1.6), we have for all $-\pi < \Phi \leq \pi$

$$|E^0_L - E^{\Phi}_L| \leq 2\Phi^2 K/L \quad \text{if } L = 2 \bmod 4 ,$$

$$|E^{\pi}_L - E^{\Phi}_L| \leq 2(\pi - \Phi)^2 K/L \quad \text{if } L = 0 \bmod 4 ,$$

and

$$|E^{\pi}_L - \mathcal{E}^{\Phi}_L(t^0_L)| \leq 4\pi^2 K/L \quad \text{if } L = 0 \bmod 4 ,$$

$$|E^{\Psi}_L - \mathcal{E}^{\Phi}_L(t^{\Psi}_L)| \leq 8\pi^2 K/L \quad \text{for all } \Psi \text{ and all even } L .$$

Because $\mathcal{E}_L^\tau$ attains its minimum E_L^τ in a dimerized configuration ($L=0 \bmod 4$), this lemma implies, for $\Phi=0$, that even if the true minimum is not dimerized, its energy differs from the best dimerized configuration by $O(1/L)$, which is two orders down from $E_L^0=O(L)$.

Proof. First note that $H(\{t_j\})$ has real matrix elements and therefore has a ground state ψ_L^0 which is *real*, and hence such that $\langle \psi_L^0 | c_{j+1,\sigma}^\dagger c_{j,\sigma} | \psi_L^0 \rangle$ is also real. Using a gauge transformation that makes $H(\{\exp(i\pi/L)t_j\})$ real one can also see that $H(\{\exp(i\pi/L)t_j\})$ has a ground state ψ_L^τ such that

$$\langle \psi_L^\tau | c_{j+1,\sigma}^\dagger c_{j,\sigma} | \psi_L^\tau \rangle = e^{i\pi/L} R_{j,\sigma} ,$$

with *real* $R_{j,\sigma}$.

Let $\{t_{L,j}^0\}$ be any minimizing configuration of $\mathcal{E}_L^0$, and let ψ_L^0 be a real ground state of $H(\{t_{L,j}^0\})$. Then, by the variational principle,

$$\begin{aligned} E_L^\Phi &\le \langle \psi_L^0 | H(\{\exp(i\Phi/L)t_{L,j}^0\}) | \psi_L^0 \rangle + \sum_j f(t_j^0) \\ &= \langle \psi_L^0 | H(\{\exp(i\Phi/L)t_{L,j}^0\}) | \psi_L^0 \rangle + \sum_j f(t_j^0) \\ &\quad + \sum_{j=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (e^{i\Phi/L}-1) t_{L,j}^0 \langle \psi_L^0 | c_{j+1,\sigma}^\dagger c_{j,\sigma} | \psi_L^0 \rangle \\ &\quad + \text{H.c.} \end{aligned}$$

The sum of the first two terms in the right side of the equality above is E_L^0. Using the reality of ψ_L^0 the last term can be estimated by $4|1-\cos(\Phi/L)|\sum_j |t_{L,j}^0|$. As $\cos x \ge 1-x^2/2$, this proves the first estimate of the lemma. The other inequalities are derived in the same way. Q.E.D.

The next lemma is an application of a version of the *Abstract Chessboard Estimate*[52] which is given in the Appendix.

Lemma 10. For any configuration of $t_j \ge 0$, with $d(t_j,t_{j+1})$ described in (1.7),

$$\begin{aligned} &\frac{1}{L}\sum_{j=1}^{L} \mathcal{E}_L^0(d(t_j,t_{j+1})) \le \mathcal{E}_L^0(\{t_j\}) \quad \text{if } L=2 \bmod 4 , \\ &\frac{1}{L}\sum_{j=1}^{L} \mathcal{E}_L^\tau(d(t_j,t_{j+1})) \le \mathcal{E}_L^\tau(\{t_j\}) \quad \text{if } L=0 \bmod 4 . \end{aligned} \tag{4.1}$$

Proof. Let $\Phi=0$ if $L=2 \bmod 4$ and $\Phi=\pi$ if $L=0 \bmod 4$. We apply Theorem 15 (with $D=\mathbf{R}^2$) to the following F:

$$F(a_1,\ldots,a_L) = \exp[-\mathcal{E}_L^\Phi(t_1,\ldots,t_L)] ,$$

where $a_j=(t_j,s_j)\in\mathbf{R}^2$. The involution R is defined by $R(t,s)=(s,t)$. The domain $\mathcal{D}$ is taken to be the set of all $(a_1,a_2,\ldots,a_L)$ of the form $((t_1,t_2),(t_2,t_3),\ldots,(t_L,t_1))$. The necessary invariance properties of $\mathcal{D}$ are trivially satisfied. The cyclicity of F follows from the invariance of $\mathcal{E}_L^\Phi$ under cyclic permutations of the t_j. The inequality of Lemma 7 translates into Schwarz's inequality for F on $\mathcal{D}$. This becomes obvious with the definitions

$$\begin{aligned} &a_1=(t_1,t_2), \quad b_1=(t_L,t_1) , \\ &a_2=(t_2,t_3), \quad b_2=(t_{L-1},t_L) , \\ &\vdots \\ &a_{L/2}=(t_{L/2},t_{L/2+1}), \quad b_{L/2}=(t_{L/2+1},t_{L/2+2}) . \end{aligned}$$

Indeed, one then has

$$\begin{aligned} &\exp[-\mathcal{E}_L^\Phi(t_1,\ldots,t_L)] \\ &\qquad = F(a_1,a_2,\ldots,a_{L/2},b_{L/2},\ldots,b_1) , \\ &\exp[-\mathcal{E}_L^\Phi(t_1,\ldots,t_{L/2},t_{L/2+1},t_{L/2},\ldots,t_2)] \\ &\qquad = F(a_1,a_2,\ldots,a_{L/2},Ra_{L/2},\ldots,Ra_1) , \\ &\exp[-\mathcal{E}_L^\Phi(t_1,t_L,\ldots,t_{L/2+2},t_{L/2+1},\ldots,t_L)] \\ &\qquad = F(Rb_1,Rb_2,\ldots,Rb_{L/2},b_{L/2},\ldots,b_1) , \\ &\exp[-\mathcal{E}_L^\Phi(t_L,t_{L-1},\ldots,t_{L/2+1},t_{L/2+2},\ldots,t_1)] \\ &\qquad = F(b_1,b_2,\ldots,b_{L/2},Rb_{L/2},\ldots,Rb_1) . \end{aligned}$$

The implication of Theorem 15, in terms of $\mathcal{E}_L^\Phi$, then reads

$$\mathcal{E}_L^\Phi(t) \ge \frac{1}{L}\sum_{j=1}^{L} \mathcal{E}_L^\Phi(t_j,t_{j+1},t_j,t_{j+1},\ldots) ,$$

which is the desired inequality. Q.E.D.

Lemma 11. For the given f let K be a constant such that $|t_{L,j}^\Phi| \le K$, for all L. For $L=0 \bmod 4$, let $\{t_{L,j}^0\}$ be any minimizing configuration of $\mathcal{E}_L^0$. Then

$$|\mathcal{E}_L^\tau(d(t_{L,j}^0,t_{L,j+1}^0)) - E_L^\tau| \le 4K\pi^2$$

for all $j=1,2,\ldots,L$.

Proof. As $L=0 \bmod 4$ we can apply Lemma 10 to $\mathcal{E}_L^\tau$ and with $t_j=t_{L,j}^0$. We then have

$$\frac{1}{L}\sum_{j=1}^{L} \mathcal{E}_L^\tau(d(t_{L,j}^0,t_{L,j+1})) \le \mathcal{E}_L^\tau(t_L^0) .$$

By Lemma 9 the right side is bounded by $E_L^\tau + 4\pi^2K/L$, and hence

$$\frac{1}{L}\sum_{j=1}^{L} \{\mathcal{E}_L^\tau(d(t_{L,j}^0,t_{L,j+1}^0)) - E_L^\tau\} \le \frac{4\pi^2K}{L} .$$

As each of the terms in the sum is non-negative, the statement of the lemma follows. Q.E.D.

Lemma 12. (i) The following limit defines a continuous function e:

$$\lim_{L\to\infty} \mathcal{E}_L^\Phi(d(x,y)) = e(x,y) .$$

The convergence is uniform on compact subsets of $\mathbf{R}^2$. (ii) If e attains its minimum at (x_0,y_0) and (y_0,x_0) and nowhere else, then there exist sequences $x_L\to x_0$ and $y_L\to y_0$ such that for all $L=0 \bmod 4$, $d(x_L,y_L)$ is a minimizing configuration for $\mathcal{E}_L^\tau$, and such that

$$\lim_{L\to\infty} \frac{1}{L}\mathcal{E}_L^\tau(d(x_L,y_L)) = e(x_0,y_0) .$$

Proof. The arguments involved in proving this lemma are fairly standard. We therefore only give a sketch of the proof.

(i) We first show that there exists a concave function $\varepsilon(x,y)$, satisfying $\varepsilon(x,y) \le 2|x|+2|y|+|U|$, and such that

$$\varepsilon(x,y) = \lim_{L\to\infty} \frac{1}{L}\lambda_0(H_L(d(x,y))) .$$

For brevity we set $G_L = \lambda_0(H_L(d(x,y)))$. By the variational principle and the fact that $\|c_{j\sigma}\|=1$ one immediately gets that G_L is "almost subadditive":

$$G_{L_1+L_2} \le G_{L_1} + G_{L_2} + 6(|x|+|y|)$$

and therefore $G_L + 6(|x|+|y|)$ is subadditive. This sequence is also almost monotone:

$$L_1 \ge L_2 \Longrightarrow G_{L_1} \le G_{L_2} + \text{const}$$

because $G_L \le 0$. It follows that the limit of G_L/L exists and as a limit of concave functions the limit is also concave. The bounds are trivial but they imply continuity and therefore the convergence is uniform on compact sets. From Lemma 9 it is obvious that e does not depend on Φ.

(ii) From the conditions on f (1.6) one has an *a priori* bound K on the minimizing t_j: $|t^{\pi}_{j,L}| \le K$. By Theorem 1, $\mathcal{E}^{\pi}_L$ always has a dimerized minimizer $d(x_L,y_L)$, and by compactness there always exists a subsequence (x_{L_k},y_{L_k}) converging to (x_*,y_*). By the continuity of e and the uniform convergence on compact sets

$$\left| \frac{1}{L_k}\mathcal{E}^{\pi}_{L_k}(d(x_{L_k},y_{L_k})) - e(x_*,y_*) \right| \to 0 .$$

As the $d(x_{L_k},y_{L_k})$ are minimizers it follows that $e(x_*,y_*) = e(x_0,y_0)$ and hence, by assumption, $(x_*,y_*)=(x_0,y_0)$ or $(x_*,y_*)=(y_0,x_0)$. Without loss of generality we can assume $x_0 \ge y_0$. Consider then the new sequence $d(\bar{x}_L,\bar{y}_L)$ of minimizers with $(\bar{x}_L,\bar{y}_L)=(x_L,y_L)$ or (y_L,x_L), and such that $\bar{x}_L \ge \bar{y}_L$ for all L. Then all convergent subsequences $(\bar{x}_{L_k},\bar{y}_{L_k})$ of $(\bar{x}_L,\bar{y}_L)$ converge to the same limit (x_0,y_0) and hence the sequence is convergent. Q.E.D.

Proof of Theorem 3(i). Let $d(x_L,y_L)$ be a sequence of minimizing configurations for $\mathcal{E}^{\pi}_L$ and such that x_L and y_L converge to x_0 and y_0, respectively, as $L\to\infty$. The existence of such a sequence is guaranteed by Lemma 12.

First we estimate $e(t^0_{L,j},t^0_{L,j+1})$ for a minimizing configuration t^0_L of $\mathcal{E}^0_L$ and any $j=1,\ldots,L$.

$$|e(t^0_{L,j},t^0_{L,j+1}) - e(x_0,y_0)| \le \left| e(t^0_{L,j},t^0_{L,j+1}) - \frac{1}{L}\mathcal{E}^{\pi}_L(d(t^0_{L,j},t^0_{L,j+1})) \right| + \frac{1}{L}|\mathcal{E}^{\pi}_L(d(t^0_{L,j},t^0_{L,j+1})) - \mathcal{E}^{\pi}_L(d(x_L,y_L))|$$
$$+ \frac{1}{L}|\mathcal{E}^{\pi}_L(d(x_L,y_L)) - e(x_0,y_0)| .$$

All three terms on the right side vanish as $L\to\infty$, uniformly in j; the first term by the uniform convergence on compact sets given by Lemma 12(i), the second by Lemma 11, and the third term by Lemma 12(ii).

The theorem now follows from the uniqueness of the dimerized minimum and compactness. Indeed, suppose one can find arbitrarily large L_k such that

$$|t^0_{L_k,j} - x| + |t^0_{L_k,j+1} - y| \ge \varepsilon ,$$

$$|t^0_{L_k,j} - y| + |t^0_{L_k,j+1} - x| \ge \varepsilon ,$$

for some $\varepsilon > 0$. By compactness and the continuity of e there would then be a limit point (x',y') of $(t^0_{L_k,j},t^0_{L_k,j+1})$, for which $e(x',y')=e(x_0,y_0)$. As (x',y') is at least distance ε away from (x_0,y_0) this would imply the existence of another minimizer for e which is ruled out by assumption. Q.E.D.

Proof of Theorem 2. Let $\Phi=0$ if $L=2 \bmod 4$ and $\Phi=\pi$ if $L=0 \bmod 4$. Denote by $d(x,y)$ the unique dimerized minimizer of $\mathcal{E}^{\Phi}_L$. Let $\{t^{\Phi}_j\}$ be any minimizer of $\mathcal{E}^{\Phi}_L$. As $\mathcal{E}^{\Phi}_L$ attains its minimum in $\{t^{\Phi}_L\}$, the inequality of Lemma 10 is an equality for $t_j = t^{\Phi}_j$. Therefore all configurations on the left side of (4.1) must be minimizers. These configurations are all dimerized and therefore (by our uniqueness assumption) must all be equal to $d(x,y)$. Q.E.D.

V. COUNTEREXAMPLES: RINGS OF LENGTH $L=0 \bmod 4$ HAVING MINIMIZERS AT ZERO FLUX THAT ARE NOT PERIOD 2

We will only discuss counterexamples with $U=0$. It is obvious, then, that counterexamples also exist with small nonvanishing U. However, the presence of a not too large on-site repulsion tends to enhance the dimerization, while nearest-neighbor repulsions can reduce it. We have not investigated the effects of interactions on the new instabilities discussed in this section. Our result for the spin-Peierls problem, Theorem 4, which can be interpreted as the $U\to\infty$ limit,[26] seems to indicate that, when U is very large, the translation symmetry can break down from period 1 to at most period 2. This seems natural because the electrons are more mobile when U is small and, under this condition, other deformations of the lattice can become favorable if the flux is not optimal. We interpret distortions that break the periodicity 2 as an attempt of the system to mimic the energy lowering effect of a nonvanishing flux. This is also a possible interpretation of the lattice distortions found in two dimensions.[45,46]

Kennedy and Lieb[18] gave an example of a function f (involving a quartic term) which gives rise to a minimum for the model on a square ($L=4$) which does *not* have periodicity 2. Longuet-Higgins and Salem pointed out

the possibility of other than period-2 instabilities a long time ago,[15] but they expected these to be unimportant and thought the period-2 instability would always dominate. They only considered the case $L=2 \bmod 4$ and therefore did not notice that other instabilities can, in fact, occur when $L=0 \bmod 4$.

Our aim in this section is twofold. First we present a family of functions f that lead to non-period-2 minimizers of the zero-flux problem for the ring of eight sites. Then we discuss what instabilities other than period 2 occur. From the discussion it will become clear how to construct many more examples of non-period-2 minima. The properties of the new instabilities, which we study partly only numerically, support our conjectures stated in the Introduction.

A. Counterexample for $L=8$

For simplicity we will present just one family of functions f chosen to yield simple values for the minimizing dimerized configuration. It is easy to generalize this example in several directions.

Define a function $f(t)$, for $t \geq 0$, as follows (see Fig. 2 for the graph of f):

$$f(t)=\begin{cases} \frac{1}{10}+\frac{1}{5}(t-1)+\frac{1}{10}(1-t)^2 & \text{if } 0 \leq t \leq 4-a \\ \frac{1}{10}+\frac{1}{5}(t-1)+\frac{1}{10}(1-t)^2+\frac{1}{3a^2}(t-4+a)^3 & \text{if } t \geq 4-a \ . \end{cases} \tag{5.1}$$

Here a can be any number strictly between 0 and $4-5/\sqrt{2} \approx 0.4645$.

Consider first configurations t_j of the form $t_{2j+1}=x, t_{2j}=y$. We always assume $x \geq y \geq 0$. The ground-state energy of eight electrons on a ring of eight sites described by the Hamiltonian (1.1) with $U=0$ is then $4e(x,y)$ where $e(x,y)$ is given by

$$e(x,y)=-x-\sqrt{x^2+y^2} \ .$$

For the 8-ring with f given in (5.1), the optimum period-2 configuration is then determined by the values of $x_0 \geq y_0$ that minimize

$$h(x,y) \equiv e(x,y)+f(x)+f(y) \ .$$

It is trivial to see that $x_0>0$, and as h is differentiable away from $x=0$ and $h(x,y) \to +\infty$ as x or $y \to +\infty$, (x_0,y_0) must therefore be a critical point of $h(x,y)$ solving the equations

$$1+\frac{x}{\sqrt{x^2+y^2}}=f'(x) \ ,$$

$$\frac{y}{\sqrt{x^2+y^2}}=f'(y) \ .$$

A straightforward calculation shows that $(x,y)=(4,3)$ is the unique minimum.

Next we study the stability of the relative minimum (x_0,y_0) under a class of perturbations which break the period-2 symmetry. For future use we do this for arbitrary $L=0 \bmod 4$, $L \geq 8$. More specifically we consider configurations of the form $t_{2j+1}=x$, $t_{2j}=y+\varepsilon V_{j+1}$, $j=1,\ldots,N \bmod N$, with $L=2N$. As we do not want to introduce a flux, the V_j must be real. One can use analytic perturbation theory to compute the energy as a function of x, y, and ε. Up to corrections of $O(\varepsilon^3)$ one finds

$$\begin{aligned} E_{\text{kin}}=&-2\sum_{n=1}^{N}\lambda_n-\varepsilon\hat{V}(0)\sum_{n=1}^{N}\frac{y+x\cos(\alpha n)}{\lambda_n} \\ &+\varepsilon^2\sum_{n=1}^{N}\left[\frac{|\hat{V}(0)|^2[y+x\cos(\alpha n)]^2}{\lambda_n^3}-\sum_{m\neq 2n \bmod N}\frac{|\hat{V}(m)|^2}{\lambda_n}\right]-\varepsilon^2\frac{|\hat{V}(0)|^2}{|x-y|} \\ &-4\varepsilon^2\sum_{n,m;\lambda_n\neq\lambda_m}|\hat{V}(n-m)|^2\frac{P_{n,m}}{\lambda_n(\lambda_n^2-\lambda_m^2)} \ , \end{aligned} \tag{5.2}$$

where E_{kin} denotes kinetic energy,

$$\lambda_n=\sqrt{x^2+y^2+2xy\cos(\alpha n)}, \quad \alpha=2\pi/N$$

and

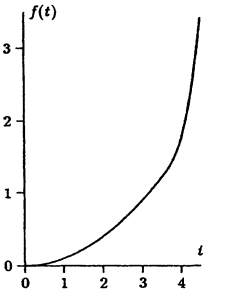

FIG. 2. Graph of the function $f(t)$ defined in (5.1) for $a=0.46$. Recall that large t corresponds to small separation w and vice versa.

$$P_{n,m}=y^2+x^2\cos[\alpha(n+m)/2]^2$$
$$+2xy\cos[\alpha(n+m)/2]\cos[\alpha(n-m)/2]\ .$$

$\hat{V}$ is the Fourier transform of V_j: $\hat{V}(q)=(1/N)\sum_j \exp(2\pi ijq/N)V_j$. Note that the coefficient of ε^2 is diagonal in $\hat{V}$. Up to terms $O(\varepsilon^3)$, the elastic energy is

$$N\left[f(y)+f(x)+\varepsilon f'(y)\sum_j V_j+\tfrac{1}{2}\varepsilon^2 f''(y)\sum_j V_j^2\right]\ .$$

In a critical point (x,y) in the set of period-2 configurations, the terms proportional to ε in the electron energy will cancel the ones in the elastic energy. A perturbation V will then lower the energy for small ε if the total (electron plus elastic energy) coefficient of ε^2 is negative, which means that the optimal dimerized configuration is not the true minimum. Call the coefficient of the ε^2 contribution to the electron energy $-\Delta(x,y)$. Note that this coefficient is always negative. There is an instability whenever

$$\Delta(x_0,y_0)>\frac{N}{2}f''(y_0)\ . \tag{5.3}$$

We now return to the model on the 8-ring and show that indeed the energy can be lowered by perturbing the dimerized minimum (x_0,y_0) found above. For the 8-ring $(N=4)$ there are four independent perturbations V_i to consider:

$$V=(1,1,1,1),\quad V=\sqrt{2}(1,0,-1,0)\ ,$$
$$V=(1,-1,1,-1),\quad V=\sqrt{2}(0,1,0,-1)\ .$$

The first, $V=(1,1,1,1)$, respects the period 2 and in the optimum dimerized configuration it cannot lower the energy. The second and the fourth have the same energy because they are translations of each other. We have normalized the V's such that $\sum_i V_i^2=4$ (in general we will use the normalization $\sum_i V_i^2=N$.) Let $-\Delta_0,-\Delta_1,-\Delta_2$ be the coefficients of ε^2 for the first, second, and third choice of V, respectively. It is convenient to factor out x as a scale factor and to use the ratio $r=y/x$ as the relevant variable, $0\le r\le 1$. The explicit expressions for the Δ's are

$$x\Delta_0=\frac{2}{(1+r^2)^{3/2}}\ ,$$
$$x\Delta_1=4-\frac{2}{\sqrt{1+r^2}}\ ,$$
$$x\Delta_2=2\ .$$

In our example both Δ_1 and Δ_2 satisfy the criterion for instability (5.3):

$$|\Delta_1(4,3)|=\tfrac{3}{5}>2f''(3)=\tfrac{2}{5}\ ,$$
$$|\Delta_2(4,3)|=\tfrac{1}{2}>2f''(3)=\tfrac{2}{5}\ .$$

Of course, $\Delta_0(4,3)$ does not satisfy (5.3), indicating that (4,3) is a stable relative minimum within the set of period-2 configurations [indeed $\Delta_0(4,3)=\frac{32}{125}<\frac{2}{5}$]. We conclude that for the choice of f defined in (5.1) the energy minimizing configuration of the 8-ring is not period 2.

B. Other than period-2 instabilities for arbitrary $L=0$ mod4

The behavior of the coefficients of ε^2 in (5.2) for large N gives support to our conjectures 1 and 2 stated in the Introduction.

Let $-\Delta_k$ denote the coefficient of ε^2 for $V=V^{(k)}(q)$, where $\hat{V}^{(k)}(q)=(\delta_{q,k}+\delta_{q,N-k})/\sqrt{2}$, $k\neq 0,N/2$, $\hat{V}^{(0)}(q)=\delta_{q,0}$, and $\hat{V}^{(N/2)}(q)=\delta_{q,N/2}$. The perturbations are normalized such that their contributions to the elastic energy are identical. Δ_0 and Δ_1 are given by

$$\Delta_0=\sum_{n=1}^{N}\frac{x^2\sin(\alpha n)^2}{\lambda_n^3}\ ,$$
$$\Delta_1=\sum_{n=1}^{N}\frac{1}{\lambda_n}+\sum_{n=1}^{N}\left[\frac{1}{\lambda_n}-\frac{1}{\lambda_{n+1}}\right]\times\frac{P_{n,n+1}}{xy\{\cos(\alpha n)-\cos[\alpha(n+1)]\}}\ .$$

The stability of a relative minimum (x_0,y_0) within the set of period-2 configurations requires that $\Delta_0<(N/2)f''(y_0)$. When $\Delta_0<(N/2)f''(y_0)<\Delta_1$ such a relative minimum is unstable against the perturbation $\varepsilon V^{(1)}$, which has wavelength equal to L. Numerical investigation of these expressions reveals the following: for $r\equiv y/x<1$ but close enough to 1 (depending on N), one has $\Delta_1>\Delta_0$. This is illustrated in Fig. 3. Note that the perturbations with $k>1$ are all stable. We showed in the preceding subsection that for $L=8$ this situation can be realized with a function f satisfying the conditions (i) and (ii) stated in the Introduction. It is reasonable to expect that this can be done for all L that are a multiple of 4, but the larger L becomes the more stringent are the restrictions on f. In particular, if one fixes f we expect that for

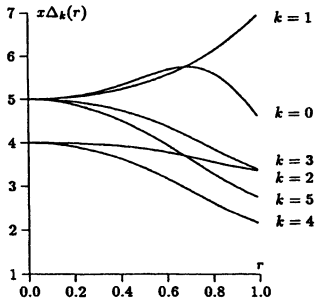

FIG. 3. Graph of the coefficients $x\Delta_k$ as a function of the ratio $r=y/x$ for $L=20$ and $k=0,\ldots,5$. An instability can occur when $\Delta_k(r)>\Delta_0(r)$. Note that this condition is satisfied only in a small region of r not much smaller than 1, and only for $k=1$, which corresponds to an instability of wavelength L in real space.

large enough systems the long wavelength instability will not occur and the system will remain in a period-2 configuration.

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APPENDIX

1. Discontinuous and nonconvex f

We have assumed throughout this paper that f was a continuous function satisfying some simple conditions as stated in the Introduction (1.6). Whether or not f is continuous we can associate a function $\bar{f}$ with f having the following properties: (a) $\bar{f}$ is convex [i.e., $\bar{f}(\lambda t+(1-\lambda)t')\le\lambda\bar{f}(t)+(1-\lambda)\bar{f}(t')$ for all $0\le\lambda\le1$ and all $t,t'\ge0$]; (b) $\bar{f}(t)=\sup\{g(t):g$ is convex and $g(t')\le f(t')$ for all $t'\ge0\}$. This function $\bar{f}$ is called the convex hull of f and is automatically continuous for $t>0$. The following lemma shows that all we really need is that $\bar{f}$ (not f) satisfy conditions (i) and (ii) of (1.6).

Lemma 13. Let $\{t_j^\Phi\}$ be a minimizing configuration of $\mathcal{E}_L^\Phi$. Then for all j, $f(t_j^\Phi)=\bar{f}(t_j^\Phi)$, where $\bar{f}$ is the convex hull of f.

Proof. Let j be arbitrary and fixed. As a function of $t_j=t$ the energy can be written as

$$\mathcal{E}(t)=E(t)+f(t)$$
$$=[E(t)+at]+[f(t)-at]=K(t)+g(t)\ .$$

We choose $a=[f(t_2)-f(t_1)]/(t_2-t_1)$ where

$$t_1=\sup\{s<t_j^\Phi|f(s)\neq\bar{f}(s)\}\ ,$$
$$t_2=\inf\{s>t_j^\Phi|f(s)\neq\bar{f}(s)\}\ .$$

As t appears linearly in the Hamiltonian H, $K(t)=E(t)+at$ is a concave function of t [i.e., $-E(t)-at$ is convex]. By construction we also have that $g(t_j^\Phi)\ge g(t_1)=g(t_2)$. Hence, with $0\le\alpha\le1$ such that $t_j^\Phi=\alpha t_1+(1-\alpha)t_2$ one has

$$\mathcal{E}(t_j^\Phi)\ge\alpha\mathcal{E}(t_1)+(1-\alpha)\mathcal{E}(t_2)$$

and the inequality is strict if $g(t_j^\Phi)=f(t_j^\Phi)-\bar{f}(t_j^\Phi)\neq0$. Therefore the minimum can be attained only at t_j where $f(t_j)=\bar{f}(t_j)$. Q.E.D.

2. The Dyson-Lieb-Simon lemma for ground states

The following lemma is a ground-state version of Lemma 4.1 in Ref. 51. An example of this ground-state version is given in Ref. 53. Note that the matrices A and B need not have real matrix elements. It is obvious how to generalize to reflections that involve an additional unitary transformation. When needed one can in fact apply the lemma as stated below after performing a unitary transformation on one-half of the system. In this paper we applied the lemma in two different situations. In the proof of Lemma 5 the two copies of the Hilbert space $\mathcal{H}$ correspond to spin up and spin down. In Lemma 7 the two spaces refer to the right and left halves of the ring.

Lemma 14. Let $A,B,C_1,\ldots,C_n$ be a collection of $d\times d$ complex matrices (n could be infinite) with the following properties: A and B are Hermitian (i.e., $A=A^\dagger,B=B^\dagger$), for all i, C_i is real, and $\sum_i C_i\otimes C_i$ is symmetric (as a $d^2\times d^2$ matrix). Let $\lambda_0(A,B)$ denote the lowest eigenvalue of the matrix

$$T(A,B)\equiv A\otimes\mathbf{1}-\sum_i C_i\otimes C_i+\mathbf{1}\otimes B\ . \tag{A1}$$

Then

$$\lambda_0(A,B)\ge\tfrac{1}{2}[\lambda_0(A,A^*)+\lambda_0(B^*,B)]\ , \tag{A2}$$

where A^* denotes the matrix obtained from A by complex conjugation of the matrix elements. In particular,

$$\lambda_0(A,B)\ge\min(\lambda_0(A,A^*),\lambda_0(B^*,B))\ .$$

The inequality (A2) is strict if for some i

$$\langle\Omega|C_i\otimes\mathbf{1}|\Omega\rangle\neq\langle\Omega|\mathbf{1}\otimes C_i|\Omega\rangle\ , \tag{A3}$$

where Ω is any eigenvector for the eigenvalue $\lambda_0(A,B)$ (this is not the only case where the inequality is strict). In particular, all ground states Ω of $T(A,A^*)$ satisfy

$$\langle\Omega|C_i\otimes\mathbf{1}|\Omega\rangle=\langle\Omega|\mathbf{1}\otimes C_i|\Omega\rangle\ .$$

Proof. Let $\{e_j\}$ be an orthonormal basis of $\mathbb{C}^d$ in which the C_i have real matrix elements. Define V to be the antilinear map leaving the e_j invariant: $Ve_j=e_j$. Then $VAV=A^*$ etc. Let Ω be an eigenvector of the smallest eigenvalue of the operator (A1) and denote by M_{ij} its coefficients in the basis $e_i\otimes e_j$:

$$\Omega=\sum_{i,j}M_{ij}e_i\otimes e_j\ .$$

We can consider (M_{ij}) as a matrix and use the eigenvectors $\{u_\alpha\}$ of $M^\dagger M$ and $\{v_\alpha\}$ of $MM^\dagger$ to define two new bases:

$$\varphi_\alpha=\sum_j\langle e_j|u_\alpha\rangle e_j,\quad\psi_\alpha=\sum_j\langle e_j|v_\alpha\rangle^* e_j\ .$$

It is then straightforward to check that

$$\Omega=\sum_\alpha\lambda_\alpha\varphi_\alpha\otimes\psi_\alpha\ .$$

We can obviously assume that $\lambda_\alpha>0$ by absorbing a phase in the definition of φ_α and by omitting any vanishing terms in the sum.

Using the fact that $\{\varphi_\alpha\}$ and $\{\psi_\beta\}$ are orthonormal bases the energy of Ω can be expressed as

$$\langle\Omega|T(A,B)|\Omega\rangle=\sum_\alpha\lambda_\alpha^2(\langle\varphi_\alpha|A|\varphi_\alpha\rangle+\langle\psi_\alpha|B|\psi_\alpha\rangle)$$
$$-\sum_i\sum_{\alpha,\beta}\lambda_\alpha\lambda_\beta\langle\varphi_\alpha|C_i|\varphi_\beta\rangle\langle\psi_\alpha|C_i|\psi_\beta\rangle\ .$$

This energy can directly be compared with the energy of $T(A, A^*)$ and $T(B^*, B)$ in the states Ω_1 and Ω_2 defined by

$$\Omega_1 = \sum_\alpha \lambda_\alpha \varphi_\alpha \otimes V\varphi_\alpha ,$$

$$\Omega_2 = \sum_\alpha \lambda_\alpha V\psi_\alpha \otimes \psi_\alpha ,$$

which have the same norm: $\|\Omega\|^2 = \|\Omega_1\|^2 = \|\Omega_2\|^2 = \sum_\alpha \lambda_\alpha^2$. The average of the energies of Ω_1 and Ω_2 is

$$\tfrac{1}{2}[\langle\Omega_1|T(A,A^*)|\Omega_1\rangle + \langle\Omega_2|T(B^*,B)|\Omega_2\rangle] = \tfrac{1}{2}\sum_\alpha \lambda_\alpha^2(\langle\varphi_\alpha|A|\varphi_\alpha\rangle + \langle V\varphi_\alpha|A^*V|\varphi_\alpha\rangle + \langle V\psi_\alpha|B^*V|\psi_\alpha\rangle + \langle\psi_\alpha|B|\psi_\alpha\rangle)$$
$$- \tfrac{1}{2}\sum_i \sum_{\alpha,\beta} \lambda_\alpha\lambda_\beta(\langle\varphi_\alpha|C_i|\varphi_\beta\rangle\langle V\varphi_\alpha|C_iV|\varphi_\beta\rangle$$
$$+ \langle\psi_\alpha|C_i|\psi_\beta\rangle\langle V\psi_\alpha|C_iV|\psi_\beta\rangle) . \qquad \text{(A4)}$$

Using $\langle V\varphi|\psi\rangle = \langle\varphi|V^\dagger|\psi\rangle^*$, for any two vectors φ, ψ, the Hermiticity of A and B, and the reality of the C_i, it is straightforward to verify

$$\langle V\varphi_\alpha|A^*V|\varphi_\alpha\rangle = \langle\varphi_\alpha|A|\varphi_\alpha\rangle ,$$

$$\langle V\varphi_\alpha|C_iV|\varphi_\beta\rangle = \langle\varphi_\alpha|C_i|\varphi_\beta\rangle^* ,$$

etc. As $\lambda_\alpha > 0$ we can then apply $2|uv| \le |u|^2 + |v|^2$ to each term in the double sum of (A4) to obtain

$$\langle\Omega|T(A,B)|\Omega\rangle \ge \tfrac{1}{2}[\langle\Omega|T(A,A^*)|\Omega\rangle + \langle\Omega|T(B^*,B)|\Omega\rangle]$$

from which (A2) directly follows by the variational principle.

The inequality is strict if for some i and some α,β, $\langle\varphi_\alpha|C_i|\varphi_\beta\rangle \neq \langle\psi_\alpha|C_i|\psi_\beta\rangle$, for which (A3) is a sufficient condition. When $A = B^*$, (A2) is an equality and so $\langle\varphi_\alpha|C_i|\varphi_\beta\rangle = \langle\psi_\alpha|C_i|\psi_\beta\rangle$ for all i,α,β in that case. Q.E.D.

From the proof of the lemma it also follows that any Hamiltonian of the form $T(A, A^*)$ has a ground state Ω satisfying

$$\langle\Omega|X\otimes X^*|\Omega\rangle \ge 0$$

for all observables X on $\mathcal{H}$.

The same state therefore also satisfies

$$\langle\Omega|X\otimes 1|\Omega\rangle = \langle\Omega|1\otimes X^*|\Omega\rangle .$$

In particular, if $[X\otimes 1, T(A,A^*)] = 0$, and $X = X^\dagger$, there will be a ground state Ω such that $X\otimes 1\Omega = 1\otimes X^*\Omega = x\Omega$ for some eigenvalue of x of X. [This also follows from application of (A2) with A replaced by $A + c(X - x_1)^2$ and B by $A^* + c(X^* - x_2)^2$, where x_1 and x_1 are the eigenvalues of $X\otimes 1$ and $1\otimes X^*$ in some ground state of $T(A, A^*)$.]

3. The Abstract Chessboard Estimate[52]

Theorem 15. Let D be a set, let $R: D \to D$ be an involution on D (R^2 = identity), and let $F: \mathcal{D} \to \mathbb{C}$ be a complex valued function on a domain $\mathcal{D} \subset D^{2N}$ that has the following invariance properties:

$$(a_1, \ldots, a_{2N}) \in \mathcal{D} \Longrightarrow (a_2, \ldots, a_{2N}, a_1) \in \mathcal{D} ,$$

$$(a_1, \ldots, a_N, b_N, \ldots, b_1) \in \mathcal{D} \Longrightarrow (a_1, \ldots, a_N, Ra_N, \ldots, Ra_1), (b_1, \ldots, b_N, Rb_N, \ldots, Rb_1) \in \mathcal{D} .$$

Assume F obeys

$$F(a_1, \ldots, a_{2N}) = F(a_2, \ldots, a_{2N}, a_1)$$

and

$$|Fa_1, \ldots, a_N, b_N, \ldots, b_1)|^2 \le F(a_1, \ldots, a_N, Ra_N, \ldots, Ra_1)F(b_1, \ldots, b_N, Rb_N, \ldots, Rb_1) .$$

Then $\|a\| \equiv |F(a, Ra, a, \ldots, Ra)|^{1/2N}$ satisfies

$$|F(a_1, .., a_{2N})| \le \prod_{j=1}^{2N} \|a_i\| .$$

The proof of the theorem is exactly the same as in Ref. 52, Theorem 4.1. In that reference it is also assumed that D is a real vector space and that F is defined on all of D^{2N}. Under these circumstances the inequality of the theorem implies that $\| \ \|$ is a seminorm on D, but we do not use this property in this paper.

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[18]T. Kennedy and E. H. Lieb, Phys. Rev. Lett. **59**, 1309 (1987). We take the opportunity to note three minor technical misstatements in this paper. (A) The paragraph after Eq. (6) is not correct for $N=2$ because $T_{13}=t_1t_2+t_3t_4$ and not t_1t_2 in this case. Thus z has to be replaced by $2z$, but the rest of the argument works. Alternatively, one can compute the eigenvalues of T^2 explicitly since it reduces to a 2×2 matrix. (B) The uniqueness proof for $N=2$ needs strengthening. $T^2=\langle T^2\rangle$ implies only that $t_1=t_3$ or $t_2=t_4$. However, this case can be analyzed explicitly and uniqueness holds. (C) The statement in *case 1* that $W(z)\equiv\mathrm{Tr}(2y^2+z\Omega)^{1/2}$ is an even function of z is correct only when N is even (because the sublattices are then themselves bipartite). However, in all cases $W(z)$ is certainly concave and $dW(z)/dz=\frac{1}{2}\mathrm{Tr}(2y^2+z\Omega)^{-1/2}\Omega$, which is zero at $z=0$. Thus $W(z)$ is decreasing for $z>0$ and increasing for $z<0$, which is what is needed in *case 1* and *case 2*.
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Part III

Falicov–Kimball Model

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A MODEL FOR CRYSTALLIZATION: A VARIATION ON THE HUBBARD MODEL

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A quantum mechanical lattice model of fermionic electrons interacting with infinitely massive nuclei is considered. (It can be viewed as a modified Hubbard model in which the spin-up electrons are not allowed to hop.) The electron–nucleus potential is "on-site" only. Neither this potential alone nor the kinetic energy alone can produce long range order. Thus, if long range order exists in this model, it must come from an exchange mechanism. N, the electron plus nucleus number, is taken to be less than or equal to the number of lattice sites. We prove the following: (i) For all dimensions, d, the ground state has long range order; in fact it is a perfect crystal with spacing $\sqrt{2}$ times the lattice spacing. A gap in the ground state energy always exists at the half-filled band point (N = number of lattices sites). (ii) For small, positive temperature, T, the ordering persists when $d \geq 2$. If T is large there is no long range order and there is exponential clustering of all correlation functions.

1. Introduction

This lecture concerns joint work with Kennedy[4]), first announced in ref. 10. It also contains some new work on the Peierls instability, not previously reported.

Much attention has been paid to the question of proving the existence of long range order in model statistical mechanical systems in which the basic atomic constituents interact with short range forces. An important example is a lattice spin system in which the spin at each site represents the localized spin of an atom located at that site and where the short range, pairwise interaction (Ising or Heisenberg) reputedly comes from an interatomic exchange energy. Another problem – so far unsolved – is the existence of periodic crystals which are supposed to come from short range (e.g., Lennard–Jones) interatomic potentials.

In the real world, however, these interactions are not given a priori; it is ultimately itinerant electrons and their correlations that give rise to the long range ordering. In other words, a deep unsolved problem is to derive magnetism or crystallization from the Schrödinger equation – or some caricature of it. The construction of a simple model based on itinerant electrons, and the rigorous derivation of ordering from it, is a challenge for mathematical physicists.

A lattice model of itinerant electrons that is believed to display ferro and antiferromagnetism – if it could be solved – is the Gutzwiller–Hubbard–

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Kanamori model[1-3]). We are also unable to solve it, but we have succeeded in proving that a simplified version of it does display crystallization. It is a toy model but it is, to our knowledge, the first example of this genre. Roughly, it has the same relation to the Hubbard model as the Ising model has to the quantum Heisenberg model. Here we shall give a brief report of our results, the full details of which will appear elsewhere[4]).

The Hubbard model, which is the motivation for our model, is defined by the second-quantized Hamiltonian

$$H^{\mathrm{H}} = \sum_{\sigma} \sum_{x,\, y \in \Lambda} t_{xy} c_{x\sigma}^{\dagger} c_{y\sigma} + 2U \sum_{x \in \Lambda} n_{x\uparrow} n_{x\downarrow}, \tag{1}$$

with the following notation: $\sigma = \pm 1$ denotes the 2 spin states of the electrons; Λ is a finite lattice; $c_{x\sigma}$ is a fermion annihilation operator for a spin σ electron at $x \in \Lambda$; $n_{x\sigma} = c_{x\sigma}^{\dagger} c_{x\sigma}$ is the number operator for spin σ at x. Electrons interact only at the same site with an energy $2U$, and $t_{xy} = t_{yx}$ is the hopping amplitude from x to y.

The crucial assumption will be made that Λ is the union of two sublattices $A \cup B$ such that $t_{xy} = 0$ unless $x \in A$, $y \in B$ or $x \in B$, $y \in A$. The number of sites in Λ, A and B are denoted by $|\Lambda|$, $|A|$ and $|B|$. The two sublattices need not be isomorphic. Thus, for example, a face-centered cubic lattice is allowed with A = face centers and B = cube corners. Λ is said to be *connected* if every $x, y \in \Lambda$ can be joined by a "path" through nonzero t's.

In our model we assume that one kind of electron (say $\sigma = -1$) does not hop. One can say that these electrons are infinitely massive. The Hamiltonian is then

$$H = \sum_{x,\, y \in \Lambda} t_{xy} c_x^{\dagger} c_y + 2U \sum_{x \in \Lambda} n_x W(x) \tag{2}$$

with $n_x = c_x^{\dagger} c_x$ (the subscript σ is omitted since the dynamic electrons have $\sigma = +1$) and with $W(x) = +1$ if a fixed electron ($\sigma = -1$) is at x and $W(x) = 0$ otherwise. It will be recognized immediately that (2) is just a fancy way to say that the moveable electrons are independent, with a single particle Hamiltonian

$$\tilde{h} = T + V, \tag{3}$$

with T being the $|\Lambda|$-square matrix t_{xy} and $V_{xy} = 2UW(x)\delta_{xy}$. It is convenient to write $\tilde{h} = h + U$ with

$$h = T + US \tag{4}$$

with $S_{xy} = s_x \delta_{xy}$, and $s_x = 1$ (resp. -1) if x is occupied (resp. unoccupied). The $\{s_x\}$ are like Ising spins.

We shall henceforth call the moveable particles "electrons" and the fixed particles "nuclei". This terminology is most appropriate if $U < 0$, for then H does represent a lattice system of electrons and nuclei in which all Coulomb interactions except the on-site electron–nucleus attraction and the on-site infinite nuclear repulsion are regarded as "screened out". This conforms with the spirit of the original Hubbard model. The electron number, the nuclear number and the total particle number, all of which commute with H, are, respectively,

$$N_e = \sum_{x \in \Lambda} n_x, \qquad N_n = \tfrac{1}{2} \sum_{x \in \Lambda} [s_x + 1] = \sum_{x \in \Lambda} W(x), \qquad \mathcal{N} = N_e + N_n. \quad (5)$$

It is to be emphasized that W does *not* represent a disordered potential. We take the "annealed", not the "quenched" system. The ground state for fixed N_e and N_n is defined by taking the ground state of H (with respect to the electrons) for each W and then minimizing the result with respect to the location of the nuclei. The ground state energy will be denoted by $E(N_e, N_n)$. Likewise, for positive temperature, we take $\mathrm{Tr}\, e^{-\beta H}$ with respect to *both* the electron variables and the nuclear locations.

Since $t_{xy} = 0$ for x, y on the same sublattice, the spectra of H and H^H are invariant under $t_{xy} \to -t_{xy}$ (all x, y). There is also a hole–particle symmetry. If $c_x^\dagger \to c_x$, $c_x \to c_x^\dagger$, $n_x \to 1 - n_x$ and $t_{xy} \to -t_{xy}$, then $H(U) \to H(-U) + 2UN_n$. If $W(x) \to 1 - W(x)$, then $H(U) \to H(-U) + 2UN_e$. A similar symmetry holds for H^H. Thus, the $U > 0$ and $U < 0$ cases are similar – from the mathematical point of view.

Our results are of two kinds. The first concerns the ground state which we prove always has perfect crystalline ordering and an energy gap (defined later). The second concerns the positive temperature ($1/kT = \beta < \infty$) grand canonical state. For large β and dimension $d \geq 2$, the long range order persists. For small β it disappears and there is exponential clustering of the nuclear correlation functions.

2. The ground state

Theorem 1. (*a*) *Let* $U < 0$. *Under the condition* $\mathcal{N} \equiv N_e + N_n \leq 2|A|$, *the ground state* (*i.e., we minimize* $E(N_e, N_n)$ *over the set* $N_e + N_n \leq 2|A|$) *occurs for* $N_e = N_n = |A|$ *and a minimizing nuclear configuration is* $W(x) = W_A(x) \equiv 1(x \in A), 0(x \notin A)$. *Under the condition* $\mathcal{N} \leq 2|B|$, *the ground state is* $N_e = N_n = |B|$ *and the B sublattice is occupied* ($W = W_B$). *If* Λ *is connected, these are the only ground states, i.e., if* $|A| > |B|$ *the ground state is unique; if* $|A| = |B|$ *it is*

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doubly degenerate. No assumption is made about the sign or magnitude or periodicity of the t_{xy} other than $t_{xy} = 0$ for $x, y \in A$ or $x, y \in B$.

(b) Let $U > 0$. Under the condition $\mathcal{N} \geq |A| + |B|$, there are two ground states: $N_e = |A|$, $N_n = |B|$, $W = W_B$ and $N_e = |B|$, $N_n = |A|$, $W = W_A$. If Λ is connected, these are the only ground states.

The condition $\mathcal{N} = |\Lambda|$ is called the *half-filled* band. If $|A| = |B| = |\Lambda|/2$, the crystal occurs at the half-filled band. If Λ is a cubic lattice, for example, this means that the ground state is a cubic lattice of period $\sqrt{2}$ oriented at 45° with respect to Λ.

Theorem 1 relies heavily on the fact that the electrons are fermions. The ground state would be completely different if they were bosons. For bosons and for Λ a cubic lattice, the nuclei would all be clumped together in the ground state instead of being spread out into a crystal. By using rearrangement inequalities it is possible to describe this clumping quantitatively.

Next, we define the *energy gap*. Actually two different definitions are of interest. First, let

$$E(\mathcal{N}) \equiv \min \{ E(N_e, N_n) | N_e + N_n = \mathcal{N} \}. \tag{6}$$

The *chemical potential* is defined by

$$\mu(\mathcal{N}) \equiv E(\mathcal{N}+1) - E(\mathcal{N}). \tag{7}$$

We say there is a *gap of the first kind* at $\mathcal{N}$ if

$$\mu(\mathcal{N}) - \mu(\mathcal{N}-1) \geq \varepsilon_1 > 0, \tag{8}$$

with ε_1 being independent of the size of the system. We say there is a *gap of the second kind* at N_e, N_n if

$$E(N_e + 1, N_n) + E(N_e - 1, N_n) - 2E(N_e, N_n) \geq \varepsilon_2 > 0. \tag{9}$$

In other words, the nuclear number is fixed in the second definition.

A gap is one indication that the system is an insulator, for it implies that it costs more energy to put a particle into the system than is gained by removing one. The first kind of gap is relevant if one views our model as an approximation to the Hubbard model; the second is relevant from the "electrons and nuclei" point of view.

Theorem 2. Assume that Λ is not only connected but that every $x, y \in \Lambda$ can be connected by a chain with $|t_{ab}| \geq \delta$ for every a, b on the chain. Also, assume that $\|T\| \leq \tau$. The following energy gaps exist with $\varepsilon_2 \geq \varepsilon_1 > 0$ and depending only on δ, τ and U:

$U < 0$: First kind at $\mathcal{N} = 2|A|$ and at $\mathcal{N} = 2|B|$. Second kind at $N_e = |A|$, $N_n = |A|$ and at $N_e = |B|$, $N_n = |B|$.

$U > 0$: First kind at $\mathcal{N} = |A| + |B|$. Second kind at $N_e = |A|$, $N_n = |B|$ and at $N_e = |B|$, $N_n = |A|$.

In order to give the flavor of our methods, the proof of Theorem 1 will be given here. The proof of Theorem 2 is more complicated.

Proof of theorem 1. Let $\lambda_1 \leq \lambda_2 \leq \cdots$ be the eigenvalues of h in (4). They depend on the nuclei. For N_e electrons the ground state energy, E, of H satisfies

$$E - UN_e = \sum_{j=1}^{N_e} \lambda_j \geq \sum_{\lambda_j < 0} \lambda_j = \tfrac{1}{2}[\operatorname{Tr} h - \operatorname{Tr}|h|]. \tag{10}$$

But $\operatorname{Tr} h = U\Sigma s_x = 2UN_n - U|\Lambda|$ and $|h| = \{T^2 + U^2 + UJ\}^{1/2}$ with $J_{xy} = t_{xy}[s_x + s_y]$. Since the function $0 < x \to x^{1/2}$ is concave, $f(y) = \operatorname{Tr}\{T^2 + U^2 + yUJ\}^{1/2}$ is concave in $y \in [-1, 1]$. But $f(-1) = f(1)$ (since $\operatorname{spec}(h)$ is invariant under $T \to -T$), so $f(1) \leq f(0)$, with equality if and only if $J \equiv 0$. Thus

$$E \geq U\mathcal{N} - \tfrac{1}{2}U|\Lambda| - \tfrac{1}{2}\operatorname{Tr}(T^2 + U^2)^{1/2}. \tag{11}$$

If Λ is connected, the only ways to have $J \equiv 0$ are either $W = W_A$ or W_B. Consider $U < 0$ and $\mathcal{N} \leq 2|A|$, whence, from (11),

$$E \geq U(2|A| - \tfrac{1}{2}|\Lambda|) - \tfrac{1}{2}\operatorname{Tr}(T^2 + U^2)^{1/2}. \tag{12}$$

If $W = W_A$ then, as is easily seen, h has precisely $|A|$ negative and $|B|$ positive eigenvalues. Thus, if $W = W_A$ and $N_e = |A|$, then (12) is an equality. The other cases are similar.

3. Grand canonical ensemble

First, we define the partition function Ξ. A nuclear configuration is denoted by $S = \{s_x\}$, $s_x = \pm 1$, and the λ_j are the eigenvalues of h in (4). If μ_n, μ_e are the nuclear and electronic chemical potentials,

$$\Xi = \sum_S \exp\left[\tfrac{1}{2}\beta\mu_n\left(\sum_x s_x + |\Lambda|\right)\right] \prod_{j=1}^{|\Lambda|} \left\{1 + \exp\left[-\beta(\lambda_j + U - \mu_e)\right]\right\}. \tag{13}$$

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The product in (13) is just the well known Fermi–Dirac grand canonical partition function for the electrons. We want to choose μ_e, μ_n so that $\langle N_e \rangle = \frac{1}{2}|\Lambda|$ and $\langle N_n \rangle = \frac{1}{2}|\Lambda|$, or $\langle \Sigma s_x \rangle = 0$. From the fact that if $T \to -T$, $\mathrm{spec}(h) \to \mathrm{spec}(h)$, one has that when $S \to -S$, $\mathrm{spec}(h) \to -\mathrm{spec}(h)$. It is then easy to see that the desired chemical potentials are $\mu_e = \mu_n = U$. Since $\Sigma\lambda_j = U\Sigma s_x$, (13) becomes in this case (after dropping an irrelevant factor $2^{|\Lambda|}/e^{\beta U|\Lambda|/2}$)

$$\Xi = \sum_S \exp[-\beta F(S)] \tag{14}$$

with

$$-\beta F(S) = \sum_{j=1}^{|\Lambda|} \ln\cosh\left(\tfrac{1}{2}\beta\lambda_j\right) = \mathrm{Tr}\ln\cosh\left[\tfrac{1}{2}\beta h\right]$$

$$= \mathrm{Tr}\ln\cosh\left[\tfrac{1}{2}\beta(T^2 + U^2 + UJ)^{1/2}\right]. \tag{15}$$

Thus, (14) is like an Ising model partition function but with a complicated, temperature dependent "spin–spin" interaction, $F(S)$, given by (15) in terms of the eigenvalues of h. With respect to this "spin measure" we can talk about the presence or absence of long range nuclear order in the thermodynamic limit. In order to discuss this limit we henceforth restrict ourselves to a translation invariant nearest neighbor hopping on a cubic lattice in d dimensions.

What we are able to prove is summarized in the schematic fig. 1 and in

Theorem 3. For all U and sufficiently large β there is long range order for $d \geq 2$ (the same kind as in the ground state). For all U and sufficiently small β there is none; indeed there is exponential decay of all nuclear correlation functions.

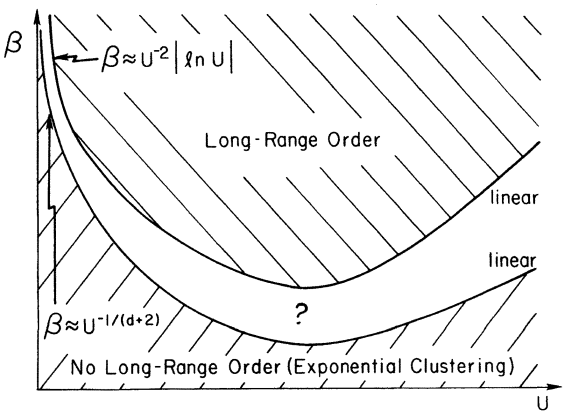

Fig. 1.

Presumably there is no intermediate phase, but we cannot prove this. For large U, β_c is clearly linear in U. For small U, we have the bound on the lower $\beta_c \sim U^{-1/(2+d)}$ and the bound on the upper $\beta_c \sim |\ln U| U^{-2}$. Our guess is that the true state of affairs is $\beta_c \sim U^{-2}$.

For large β we use a Peierls argument; for small β we use Dobrushin's uniqueness theorem. A sketch of our proof – omitting many important details – is the following. For simplicity, we here consider only large $U > 0$.

Define, for $x > 0$,

$$P(x) = \ln \cosh x^{1/2}. \tag{16}$$

[We note in passing that P is concave, and we see from the last expression in (15), using the proof in Theorem 1, that $F(S)$ has its minima at precisely the same values of W (or S) as in Theorem 1.] P is a Pick (or Herglotz) function with the representation

$$P'(x) = \tfrac{1}{2} x^{-1/2} \tanh x^{1/2} = \sum_{k=0}^{\infty} \left[\left(k + \tfrac{1}{2}\right)^2 \pi^2 + x \right]^{-1}. \tag{17}$$

We are interested in $x = \frac{1}{4}\beta^2(T^2 + U^2 + UJ)$ with $J_{xy} = t_{xy}(s_x + s_y)$.

Long range order (large β)

Choose S, and then define antiferromagnetic contours in the usual way. If γ is a connected contour component and $\Gamma + \gamma$ is the whole contour, we want to prove that $\Delta \equiv F(\Gamma + \gamma) - F(\Gamma) \geq C|\gamma|$ for a suitable constant $C = C(U)$.

Obviously, $J_{\Gamma+\gamma} = J_\Gamma + J_\gamma$. To remove γ, we change s_x to $-s_x$ inside γ. For $0 \leq t \leq 1$, define $J(t) = J_\Gamma + tJ_\gamma$. Then, assuming for simplicity that Γ lies entirely outside γ, we have, by differentiating (15) and using (17), that

$$-\beta\Delta = \tfrac{1}{4}\beta^2 U \sum_{k=0}^{\infty} \int_0^1 \mathrm{d}t \, \mathrm{Tr}\left(G_k J_\gamma\right), \tag{18}$$

with

$$G_k = \left[\left(k + \tfrac{1}{2}\right)^2 \pi^2 + \tfrac{1}{4}\beta^2 \left(T^2 + U^2 + UJ_\Gamma + tUJ_\gamma\right) \right]^{-1}. \tag{19}$$

Integrating by parts, this becomes

$$-\beta\Delta = -\left(\beta^4 U^2/16\right) \sum_k \int_0^1 \mathrm{d}t \, (1-t) \, \mathrm{Tr}\, G_k J_\gamma G_k J_\gamma + \cdots. \tag{20}$$

[The $\cdots$ terms in (20) come from $t = 0$ in the partial integration. They are small

and easily bounded for large U, but they have to be treated more judiciously when U is small.] If A, B, D are matrices with $A \geq B \geq 0$, then $\mathrm{Tr}\, AD^{\dagger}AD \geq \mathrm{Tr}\, BD^{\dagger}BD$. Also, $A \geq B > 0 \Rightarrow 0 < A^{-1} \leq B^{-1}$. Moreover, $T^2 \leq (2d)^2$ and $UJ \leq T^2 + U^2$. Using this, we have the matrix inequality

$$G_k \geq \left[\left(k + \tfrac{1}{2}\right)^2 \pi^2 + \tfrac{1}{2}\beta^2\left((2d)^2 + U^2\right)\right]^{-1}. \tag{21}$$

Summing on k,

$$\Delta \geq (\text{const.})U^2\left((2d)^2 + U^2\right)^{-3/2}\mathrm{Tr}\left(J_\gamma\right)^2.$$

Clearly $\mathrm{Tr}\,(J_\gamma)^2 = (\text{const.})|\gamma|$. Thus, for U large, $C(U) \geq (\text{const.})U^{-1}$, and thus long range order exists in $d \geq 2$ if β/U is large enough.

Absence of long range order (small β)

Dobrushin's uniqueness theorem[5-7]), together with the modification in[8]), gives the following criterion for exponential clustering. We have to bound the change in F when we change the spins at x and y (taking the worst case with respect to the other spins). Call this f_{xy}. The requirement is that for some $m > 0$ and all x,

$$\beta \sum_y f_{xy} \exp\left[m|x - y|\right] < 1. \tag{22}$$

By an argument similar to the preceding (large U)

$$f_{xy} \cong \left(\beta^3 U^2/16\right)\sum_k \mathrm{Tr}\, G_k J_x G_k J_y$$

$$\cong \left(\beta^3 U^2/16\right)\sum_k |G_k(x, y)|^2. \tag{23}$$

Here, $J_x = \delta_x T + T\delta_x$ and $G_k(x, y)$ is the x, y matrix element of (19).

To implement (22) we now require an *upper* bound on $G_k(x, y)$ that has exponential decay. For this purpose the Combes–Thomas[9]) argument is ideal. Let Q be the matrix with elements $Q_{xy} = \delta_{xy}\, e^{n \cdot x}$ and with $|n| = 1$. Then

$$QG_k^{-1}Q^{-1} = G_k^{-1} + R_k \equiv L_k. \tag{24}$$

The "remainder" R_k can be bounded for large U: $\|R_k\| \leq C\beta^2 U$ for some constant C. Similar to (21), for large U

$$G_k^{-1} \geq \left[\left(k + \tfrac{1}{2}\right)^2 \pi^2 + \tfrac{1}{8}\beta^2 U^2\right] \equiv \alpha_k. \tag{25}$$

Thus,

$$\|L_k^{-1}\| \leq \left[\alpha_k - C\beta^2 U\right]^{-1}. \tag{26}$$

Since $|(L_k^{-1})_{xy}| \leq \|L_k^{-1}\|$, we have from (24), $|(QG_kQ^{-1})_{xy}| \leq \|L_k^{-1}\|$, and thus

$$|(G_k)_{xy}| \leq \exp\left[n \cdot (y - x)\right]\left\{\alpha_k - C\beta^2 U\right\}^{-1}. \tag{27}$$

This holds for all n, no summing on k,

$$f_{xy} \leq (\text{const.})U^{-1}\mathrm{e}^{-2|x-y|}.$$

Hence (22) holds with $m = 1$ if β/U is small enough.

4. The Peierls instability

Another itinerant electron model in which translation invariance is partially broken was introduced by Peierls[11]); see also ref. 14. Consider a linear chain of $2N$ atoms (arranged in a ring) and let w_i $(i = 1, \ldots, 2N)$ denote the distance from atom i to atom $i + 1$ (with $2N + 1 \equiv 1$). If $d > 0$ is the equilibrium distance, the distortion energy associated with the w_i is taken to be

$$U(\{w\}) = \kappa \sum_{i=1}^{2N} (w_i - d)^2. \tag{28}$$

Here $\kappa > 0$ is a measure of stiffness.

Now suppose there are $2N$ (spin $\frac{1}{2}$) electrons ($\frac{1}{2}$ filled band) which can hop between nearest neighbor atoms, with an amplitude $t_i = t(w_i)$ to hop from atom i to $i + 1$ and from $i + 1$ to i. The function $t(w)$ will be explained shortly. The ground state energy of these $2N$ electrons is

$$K(\{w\}) = 2 \sum_{j=1}^{N} \lambda_j(T), \tag{29}$$

where $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{2N}$ are the eigenvalues of the $2N \times 2N$ matrix T having matrix elements $T_{i,i+1} = T_{i+1,i} = t_i = t(w_i)$ and $T_{ij} = 0$ otherwise. The total Hamiltonian is

$$H(\{w\}) = K(\{w\}) + U(\{w\}) \tag{30}$$

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and the problem is to determine the ground state energy

$$E = \min_{\{w\}} H(\{w\}) \tag{31}$$

and the configuration(s) $\{w\}$ that attains it.

The function $t(w)$ should be something like $a\,e^{-cw}$, but here we shall adopt the choice of Su, Schrieffer and Heeger[12]):

$$t(w) = b - c(w - d) \tag{32}$$

with $b, c > 0$.

One guess for a minimizing $\{w\}$ is $w_i = W = \text{const}$. However, Peierls observed that if we take $w_i = W + (-1)^i\delta$ (a *dimerized configuration*) the energy will be lowered. The reason is that when $\{w\}$ has period two, a gap in the spectrum of T opens up at $k = \pm\pi/2$; since there are just enough electrons to fill the lower band, the K energy will be lowered by an amount (const.) $\delta^2 \ln|\delta|$ for small δ. (This comes from the fact that the perturbation theory is singular at the band edges.) On the other hand, U depends on δ like $\kappa\delta^2$, so it is favorable to have $\delta \neq 0$. This breaking of translation invariance is called the Peierls instability. The interesting question, which was open for a long time, is this: Is the translation invariance merely broken from period one to period two, or does something more complicated happen? Conceivably the minimizing $\{w\}$ could have a longer period – or perhaps no periodicity at all.

Our answer to this question is that period two always holds.

Theorem 4. For all b, c, d, κ, N there are precisely two minima for E,

$$w_i = W + (-1)^i\delta \quad \textit{or} \quad w_i = W - (-1)^i\delta, \tag{33}$$

with W and δ being constants depending on κ, b, c, N. Moreover, there is a gap, i.e., a jump in the chemical potential:

$$\Delta\mu \equiv [E(2N+1) - E(2N)] - [E(2N) - E(2N-1)] > \varepsilon, \tag{34}$$

with ε depending on κ, b, c but independent of N, d. (Here $E(2N+1)$ is defined as in (30) and (31) but with K replaced by $2\Sigma_{j=1}^{N}\lambda_j(T) + \lambda_{N+1}(T)$ and, for $E(2N-1)$, K is replaced by $2\Sigma_{j=1}^{N}\lambda(T) - \lambda_N(T)$.)

As in the proof of Theorem 1, the proof of Theorem 4 uses the concavity of $\mathrm{Tr}\sqrt{X}$ with respect to X, and with $X = T^2$. The crucial observation is that for the dimerized configuration (33), T^2 is translation invariant.

It turns out that if the U in (28) is modified, an "integrable system" is obtained. In terms of t, using (32), we have

$$(w_i - d)^2 = \alpha + \beta t_i + \gamma t_i^2, \tag{35}$$

with α, β, γ constants. The modification is

$$U(\{w\}) = \alpha + \sum_{j=1}^{2N} \left[-\beta \ln t_i + \gamma t_i^2 \right], \tag{36}$$

with α, β, γ arbitrary constants (but (32) is unchanged). This system is presumably not very different from ours (but there is no proof). It was investigated in ref. 13. However, the solution in ref. 13 covers all electron numbers *except* the half-filled band ($2N$ electrons), which is the most interesting case since it is only here that one expects to see the instability manifest itself in the form proposed by Peierls – namely the partial breaking of translation invariance into a period two invariance.

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Phase Separation due to Quantum Mechanical Correlations

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Can phase separation be induced by strong electron correlations? We present a theorem that affirmatively answers this question in the Falicov-Kimball model away from half filling, for any dimension. In the ground state the itinerant electrons are spatially separated from the classical particles.

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The Falicov-Kimball (FK) model [1] can be viewed as a modification of the Hubbard (H) model [2] in which one species of electrons (say spin down) has infinite mass. As such, its relation to the latter is similar to the relation of the Ising model to the quantum Heisenberg model [3,4]. Alternatively, it can be viewed as a model of itinerant electrons and immobile ions. It possesses long range order at low temperature in two or more dimensions at half filling, and this checkerboard state (and higher-period generalizations [5–8]) remain to date as the only examples of crystallization into a perfectly ordered structure whose periodicity is not that of the underlying lattice.

In this paper, we report a theorem on the existence of phase separation in the ground state of the FK model, away from half filling and for large repulsion between the particles. "Phase separation," or "segregation," means that the system splits into two large domains, one being occupied by the classical particles, and the other by the quantum particles. In the language of the H model, this would mean segregation of spin up particles from spin down particles—resulting in a ferromagnetic state. The question of whether strong interactions can drive quantum (electronic) systems to phase separate was posed over ten years ago for the FK model [9] and the H model [10]. This work is a rigorous proof of this long-standing conjecture for the FK model. Further discussion of the relation between the FK and the H models is given later.

Phase separation is not new in classical lattice models. It is present in the Ising model, and in many other classical models. It also occurs in the FK model at half filling for some densities, as was proved in [7]. In these examples, it is mainly a *local* phenomenon: interactions (or "effective interactions" in the case of FK) tend to dislike boundaries, and the state with minimum boundary is phase separated.

The electrons of the FK model are in delocalized wave functions, and away from half filling their energy cannot be written as a sum of local terms. While we prove that the ground state energy is roughly proportional to the boundary between occupied and empty sites, the mechanism is *nonlocal* and genuinely quantum mechanical.

The FK Hamiltonian [1] is

$$H = -\sum_{\mathbf{x},\mathbf{y}\in\Omega} t(\mathbf{x}-\mathbf{y}) c_{\mathbf{x}}^{\dagger} c_{\mathbf{y}} + U \sum_{\mathbf{x}\in\Omega} c_{\mathbf{x}}^{\dagger} c_{\mathbf{x}} w_{\mathbf{x}}. \quad (1)$$

Here, $t(\mathbf{x}-\mathbf{y}) = t(\mathbf{y}-\mathbf{x})$ is the hopping coefficient between sites $\mathbf{x}$ and $\mathbf{y}$; it is translation invariant, but may depend on the direction (this allows consideration of general Bravais lattices). $c_{\mathbf{x}}^{\dagger}$ and $c_{\mathbf{x}}$ are creation and annihilation operators for a spinless electron at site $\mathbf{x}$, and $w_{\mathbf{x}} = 1$ or 0 is a classical variable that denotes the presence or the absence of an ion at $\mathbf{x}$. (Spin degrees of freedom have trivial behavior and are left aside here.) $\Omega \subset \mathbb{Z}^d$ is a finite d-dimensional lattice, and U is the on-site repulsion between the two species of particles. For any given configuration $w = \{w_{\mathbf{x}}\}$ of classical particles, the ground state for N_e electrons is determined by diagonalizing a one-body operator given by the above Hamiltonian, and filling in the lowest N_e states. The main question is to find which configuration w, with a given number of classical particles $N_c = \sum_{\mathbf{x}} w_{\mathbf{x}}$, minimizes the energy of the electrons.

Our theorem states upper and lower bounds for the energy of N_e electrons, for a given configuration w of the classical particles. For orientation, let us consider first a configuration where the sites devoid of classical particles form a large, "compact" region. The expected energy of the electrons is a bulk term that scales like the volume of this region, and a correction that scales like its boundary. Our main result is a proof of this conjecture for *all* configurations, not only "nice" ones.

We need some notation. Let $\Lambda = \{\mathbf{x} \in \Omega : w_{\mathbf{x}} = 0\}$ denote the set of empty sites for the configuration w, and $\partial\Lambda$ its boundary, $\partial\Lambda = \{\mathbf{x} \in \Lambda, \mathrm{dist}(\mathbf{x}, \Omega \setminus \Lambda) = 1\}$. Their respective number of sites are $|\Lambda|$ and $|\partial\Lambda|$. We write $E(N_e, w)$ for the ground state energy of N_e electrons in the configuration w. An important quantity is $n = n_e/(1-n_c)$, where $n_e = N_e/|\Omega|$ and $n_c = \sum_{\mathbf{x}} w_{\mathbf{x}}/|\Omega|$ are the densities for quantum and classical particles, respectively. It represents the electronic density that would

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exist inside Λ, if all electrons live inside the domain devoid of classical particles. Let $e(n)$ be the usual kinetic energy per site for noninteracting electrons with density n in the thermodynamic limit [its expression is recalled below, see Eq. (4)].

THEOREM: For all Λ we have upper and lower bounds, $e(n)|\Lambda| + \alpha'(n)|\partial\Lambda| \geq E(N_e, w) \geq e(n)|\Lambda| + \alpha(n, U)|\partial\Lambda|$.

For nearest-neighbor hoppings [i.e., $t(\mathbf{x}) \neq 0$ if $|\mathbf{x}| = 1$, $t(\mathbf{x}) = 0$ otherwise], $\alpha(n, U) = \alpha(n) - \gamma(U)$, where $\alpha(n) = \alpha(1 - n)$ is strictly positive for $0 < n < 1$, and $\gamma(U)$ satisfies $\lim_{U\to\infty} U\gamma(U) = 8d^2$.

The theorem clearly leads to segregation because low-energy configurations must have a small boundary, i.e., there is a relatively small number of empty sites that are neighbors of the classical particles. Furthermore, due to the large repulsion, electrons are essentially located in the empty domain. The boundary of the configuration of classical particles that minimizes the energy is smaller than the minimum possible boundary times the ratio between the upper and lower bounds $\alpha'(n)/\alpha(n, U)$, which is a large number.

One can state an explicit bound in the case of n small, or close to 1. We assume that the (nearest neighbor) hoppings satisfy $1 \leq t(\mathbf{x}) \leq t_{\mathrm{m}}$, and we set $t = \frac{1}{2}\sum_{|\mathbf{x}|=1} t(\mathbf{x})$. Then for $n < n_0 = |S_d|/(4\pi)^d t_{\mathrm{m}}$, we can choose

$$\alpha(n) = \frac{2^{d-3}}{\pi^d |S_d|^{2/d} t^3 t_{\mathrm{m}}^{d/2}} n^{1+(2/d)}. \tag{2}$$

Here, $|S_d|$ is the volume of the d-dimensional unit sphere. Since the hypercubic lattice is bipartite the Hamiltonian has a symmetry, so that $\alpha(1 - n) = \alpha(n)$; the equation above then leads to a bound for $n > 1 - n_0$. The case $n_0 < n < 1 - n_0$ turns out to be considerably more difficult to handle, and our bound for $\alpha(n)$ is much smaller; see [11].

Our theorem is proved only in the case of the hypercubic lattice $\mathbb{Z}^d$. The results should also hold for other lattices, however, the partial proof below is clearly very general.

Phase separation in the FK model for large U was conjectured in [9] and is in stark contrast to the situation at $n_c = n_e = \frac{1}{2}$, where long-range order of checkerboard type occurs, as was established in [3,4]. The theorem is proved in [11], and extends results for $d = 1$ [12] and $d = \infty$ [13] to all dimensions, in particular to the dimensions 2 and 3 that are of great physical relevance. Its proof relies on a result of Li and Yau for the Laplace operator in the continuum [14] (see also [15], theorem 12.3). We explain this elegant proof below in the case of a lattice, thereby proving the lower bound for $U = \infty$ without the boundary correction. To include this boundary correction requires considerably more effort, and we refer to [11] for further details.

Proof with $\alpha(n) = 0$ and $U = \infty$: The ground-state energy $e(n)$ for noninteracting electrons with density n is found in the usual fashion: (i) define a Fermi energy ε_{F} via

$$\frac{1}{(2\pi)^d}\int_{\epsilon(\mathbf{k})\leq\varepsilon_{\mathrm{F}}} d^d k = n, \tag{3}$$

with the band structure $\epsilon(\mathbf{k}) = -\sum_{\mathbf{x}} t(\mathbf{x})\exp(-i\mathbf{k}\cdot x)$ and (ii) do the integration

$$\frac{1}{(2\pi)^d}\int_{\epsilon(\mathbf{k})\leq\varepsilon_{\mathrm{F}}} \epsilon(\mathbf{k}) d^d k = e(n). \tag{4}$$

The electrons are forbidden to lie on any site occupied by the classical particles. Then the eigenfunctions for a given configuration w are found by diagonalizing the projection of the hopping matrix onto Λ. Let $\phi_\beta(\mathbf{y}; w)$ denote the orthonormal eigenvectors of the Hamiltonian indexed by $\beta = 1, \ldots, |\Omega| - N_c$ for the configuration w with eigenvalues $\epsilon_\beta(w)$. We choose the ordering of the labels such that $\epsilon_1(w) \leq \epsilon_2(w) \leq \ldots \leq \epsilon_{|\Omega|-N_c}(w)$. We also extend the definition of the eigenvectors to all of $\mathbb{Z}^d$ setting $\phi_\beta(\mathbf{y}; w) = 0$ for all $\mathbf{y}\notin\Omega$. The ground state energy for N_e electrons and N_c classical particles in the configuration w is

$$E(N_e, w) = \sum_{\beta=1}^{N_e} \epsilon_\beta(w), \tag{5}$$

and the ground-state energy $E_{\mathrm{g.s.}}(N_e, N_c)$ is the minimum of Eq. (5) over all configurations that contain N_c classical particles.

Using the definition of the eigenvectors allows us to write the ground state energy as

$$E(N_e, w) = \sum_{\beta=1}^{N_e}\sum_{\mathbf{y},\mathbf{z}\in\mathbb{Z}^d} \phi_\beta^*(\mathbf{y}; w)[-t(\mathbf{y} - \mathbf{z})]\phi_\beta(\mathbf{z}; w). \tag{6}$$

Now, we define the Fourier transform of the eigenfunctions by

$$f_\beta(\mathbf{k}; w) = \sum_{\mathbf{y}\in\mathbb{Z}^d} e^{i\mathbf{k}\cdot\mathbf{y}}\phi_\beta(\mathbf{y}; w), \tag{7}$$

for every wave vector $\mathbf{k}$ in the Brillouin zone $[0, 2\pi]^d$. It is well known that the energy can be expressed as

$$E(N_e, w) = \frac{1}{(2\pi)^d}\int d^d k \epsilon(\mathbf{k})\rho(\mathbf{k}; w); \tag{8}$$

here and in the following the integral is over $[0, 2\pi]^d$ and we introduced the density function

$$\rho(\mathbf{k}; w) = \sum_{\beta=1}^{N_e} |f_\beta(\mathbf{k}; w)|^2. \tag{9}$$

The density function is obviously positive and is bounded above by $|\Lambda|$. Indeed, we can write

$$\rho(\mathbf{k}; w) = \sum_{\beta=1}^{N_e}\sum_{\mathbf{y},\mathbf{z}\in\mathbb{Z}^d} e^{-i\mathbf{k}\cdot\mathbf{z}}\phi_\beta^*(\mathbf{z}; w)e^{i\mathbf{k}\cdot\mathbf{y}}\phi_\beta(\mathbf{y}; w); \tag{10}$$

this can be rewritten as

$$\rho(\mathbf{k};w) = \sum_{\mathbf{y},\mathbf{z}\in\Lambda} e^{-i\mathbf{k}\cdot\mathbf{z}}\rho(\mathbf{z},\mathbf{y};w)e^{i\mathbf{k}\cdot\mathbf{y}}, \qquad (11)$$

with $\rho(\mathbf{z},\mathbf{y};w) = \sum_{\beta=1}^{N_e}\phi_\beta^*(\mathbf{z};w)\phi_\beta(\mathbf{y};w)$. The matrix ρ is a positive semidefinite matrix bounded by 1 (it is the projector onto the lowest N_e eigenvectors). Hence,

$$\rho(\mathbf{k};w) \le \sum_{\mathbf{y}\in\Lambda} |e^{i\mathbf{k}\cdot\mathbf{y}}|^2 = |\Lambda|. \qquad (12)$$

Furthermore, the density function satisfies a sum rule

$$\frac{1}{(2\pi)^d}\int d^dk\rho(\mathbf{k};w) = \sum_{\mathbf{y}\in\Lambda}\rho(\mathbf{y},\mathbf{y};w) = N_e. \qquad (13)$$

One gets a lower bound for $E(N_e,w)$ by minimizing the right side of (8) over all functions ρ satisfying $0 \le \rho \le |\Lambda|$ and whose integral is N_e. This is the "bathtub principle," see [15], theorem 1.14; the minimizer is $\rho(\mathbf{k}) = |\Lambda|$ for $\{\mathbf{k}: \epsilon(\mathbf{k}) \le \varepsilon_F\}$ and $\rho(\mathbf{k}) = 0$ otherwise, with ε_F defined by Eq. (4). This amounts to filling the lowest eigenvalues of the infinite lattice.

The proof of the upper bound for the energy proceeds by forming an "average" Hamiltonian by translating and rotating the original configuration w over a large but finite subset of $\mathbb{Z}^d$ (with periodic boundary conditions). Then on a bipartite lattice one can show by concavity of the sum of the lowest N eigenvalues of a matrix that the averaged Hamiltonian provides an upper bound to the ground state energy. But the magnitude of the averaged hopping is determined by the size of the boundary, which eventually yields the desired upper bound. Extending the proof above to provide the lower bound is much more complicated and relies on a detailed technical examination of the influence of the boundary sites on the minimal density function for a given configuration of classical particles. It is done in the isotropic case (that is, a hypercubic Bravais lattice with equal hoppings in all directions) in [11]; the extension to the anisotropic case is straightforward, but numerous details are modified, and have been verified.

The results of the theorem have a number of implications for the FK model. It establishes that segregation occurs in all dimensions (at $T = 0$ and $U = \infty$), illustrating the fact that the existence of periodic ground states requires a subtle reduction in energy relative to the segregated phase as the interaction strength is made finite. Since the electronic wave functions will be exponentially localized within Λ, the results shown here can be extended to the case of finite interaction strength, as long as U is large enough. At positive temperature it is so far impossible to claim rigorous results, except the following weaker one: the electronic free energy (for a *fixed* configuration of classical particles) can be shown to be equal to the bulk free energy plus a correction term that is proportional to the size of the boundary. We expect that the coexistence of two phases occurs at finite temperature for $d \ge 2$ as it happens in the Ising model.

It may be instructive to consider the $U = \infty$ results for the FK model as a guide for possible behavior in the H model. To do this, we must first find a way to interpolate between the two models. The simplest way is to consider an asymmetric-hopping H model where the hopping for the spin-up and the spin-down particles is different. Then the H model results when $t_\uparrow = t_\downarrow$ and the FK model when $t_\downarrow = 0$. Our rigorous results only hold for $t_\downarrow = 0$. When $t_\downarrow$ is increased the classical particles should still be packed, due to the pressure of the electrons. When $t_\downarrow$ keeps increasing, however, the classical particles should be in a phase with density strictly less than 1. The central issue is whether the reduction of the down-spin kinetic energy can be made large enough, so that the phase separation disappears at a critical value of $t_\downarrow$. If this occurs for all electron densities, there is no (saturated) ferromagnetism in the $U = \infty$ H model on the given lattice, however, one has a saturated ferromagnetic ground state if the phase separation survives [note the SU(2)-imposed degeneracy of the ferromagnetic multiplet will occur precisely at $t_\downarrow = t_\uparrow$]. It is well known that ferromagnetism depends strongly on the geometry of the lattice [16,17], so the occurrence of a critical value of $t_\downarrow$ must also depend strongly on the geometry of the lattice. We are unable to make any rigorous statements about ferromagnetism in the H model here; actually, we do not even know how to study the case with nonzero, but small $t_\downarrow$.

A major question is what happens to the chessboard phase when doped away from half filling? Consider the line $n_e = n_c$; the chessboard phase is present when these densities are equal to $\frac{1}{2}$, and segregation takes place when they differ significantly from $\frac{1}{2}$ (depending on U). It is not clear what to expect for intermediate values. Two possible scenarios are (i) the coexistence between chessboard and segregated phases or (ii) the coexistence between other periodic and segregated phases. Both scenarios could be of physical relevance to stripe physics.

We conclude this Letter by a summary of our knowledge of the phase diagram for zero temperature and $d \le 2$ (see Ref. [18] for a review). Recall that the particle-hole symmetry implies that the phase diagram is symmetric under the transformation $(n_e, n_c) \mapsto (1 - n_e, 1 - n_c)$ [3]. We describe the situation only for $n_e + n_c \le 1$.

In two dimensions, the ground states are *periodic* when (i) $(n_e, n_c) = (\frac{1}{2}, \frac{1}{2})$ (they are of the chessboard type). This was proved for all U in [3]; (ii) $n_c = 1 - n_e$ (i.e., at half filling), and $n_e = \frac{2}{5}, \frac{1}{3}, \frac{1}{4}, \frac{2}{9}, \frac{1}{5}, \frac{2}{11}, \frac{1}{6}$; also, $n_e = \frac{1}{n^2+(n+1)^2}$ with integers n. This holds for U large enough (depending on n_e), and follows from [5–7,19,20]; (iii) $n_c = 1 - n_e$, and the electronic density n_e is a rational number between $\frac{1}{3}$ and $\frac{2}{5}$. U must be larger than a value that depends on the denominator of n_e [8].

There is *coexistence* of two periodic phases when $n_c = 1 - n_e$ and $n_e \in (\frac{1}{6}, \frac{2}{11}) \cup (\frac{1}{5}, \frac{2}{9}) \cup (\frac{2}{9}, \frac{1}{4})$, for U large [7,19]; and the ground states display *segregation*

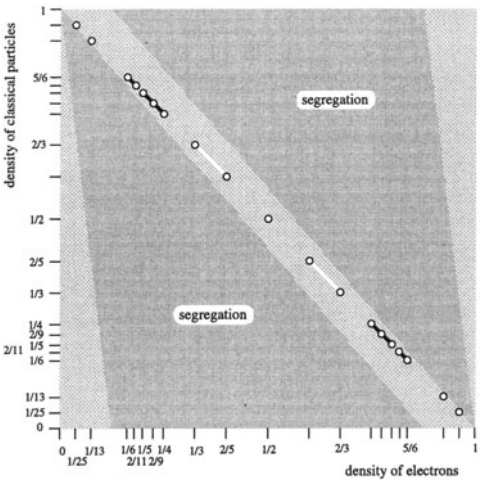

FIG. 1. Schematic phase diagram of the rigorous results for the ground state of the 2D Falicov-Kimball model for large U. The white dots and the white lines represent periodic phases; the black lines are coexistences between different periodic phases; the dark gray regions are segregated. There are no rigorous results for light gray domains.

for $\frac{\text{const}}{U}(1-n_c) < n_e < (1-\frac{\text{const}}{U})(1-n_c)$; this is described here and proved in [11].

These results are illustrated in Fig. 1. The domain $\frac{\text{const}}{U}(1-n_c) > n_e$ should also be segregated. The central band that includes the line $n_e + n_c = 1$ should be the host of numerous periodic phases and various coexistences between periodic phases and empty or full phases. This is supported by numerical simulations in 2D [21].

In one dimension, the ground states are *periodic* when $(n_e, n_c) = (\frac{1}{2}, \frac{1}{2})$ [3] and when $n_c = 1 - n_e$ (half filling) and $n_c = p/q$ is a rational number (in an irreducible fraction). The periodicity is q for U sufficiently large (depending on q) [12].

For finite U, there is numerical evidence for *coexistence* of two periodic phases and free electrons when $n_c = 1 - n_e$, $p/q < n_c < p'/q'$, and the periodic phases with periods q and q' are the only stable phases within the above interval [22]; and the ground states display *segregation* when $n_e \neq 1 - n_c$ and U is sufficiently large [11,12]. The canonical phase diagram for small U is even richer, but our knowledge of it is very limited [23,24].

In conclusion, we have proved that the FK model is phase separated whenever $N_e < |\Lambda|$ and $U \to \infty$. This shows how strong correlations can lead to phase separation.

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Part IV

Ordering of Energy Levels

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Theory of Ferromagnetism and the Ordering of Electronic Energy Levels

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Consider a system of N electrons in one dimension subject to an arbitrary symmetric potential, $V(x_1,\cdots,x_N)$, and let $E(S)$ be the lowest energy belonging to the total spin value S. We have proved the following theorem: $E(S)<E(S')$ if $S<S'$. Hence, the ground state is unmagnetized. The theorem also holds in two or three dimensions (although it is possible to have degeneracies) provided $V(x_1,y_1,z_1;\cdots;x_N,y_N,z_N)$ is separately symmetric in the x_i, y_i, and z_i. The potential need not be separable, however. Our theorem has strong implications in the theory of ferromagnetism because it is generally assumed that for certain repulsive potentials, the ground state is magnetized. If such be the case, it is a very delicate matter, for a plausible theory must not be so general as to give ferromagnetism in one dimension, nor in three dimensions with a separately symmetric potential.

INTRODUCTION

THIS paper consists mainly in the enunciation and proof of a theorem about the ordering of the energy levels of a system of interacting fermions. As such, our primary concern is with mathematics. Without striving to be pedantic, we have endeavored to construct the proof with care and rigor.

We take advantage of the symmetry properties of electron wave functions belonging to various values of total spin-angular-momentum S. In certain cases we are able to order the ground-state energies belonging to the various spins without any explicit numerical calculations. This circumvents the great difficulties of the N-body problem, such as the applicability of perturbation theory, etc.

Our theorem is not without some theoretical consequences. Notably, whenever it is applicable, there can be no ferromagnetism unless one postulates explicitly spin- or velocity-dependent forces. (The theorem does not apply to electrons in a three-dimensional lattice interacting with Coulomb or central forces; but conversely, correct theories of ferromagnetism should not predict ferromagnetism for interactions which *are* covered by the theorem.) However, as the mathematics stand quite independently of such applications, we shall defer further considerations of the physical consequences of this work to the end of the paper (Sec. IV).

In Sec. I we shall state and prove the theorem for a one-dimensional electron system. In order to pass to higher dimensions, it will be necessary to prove further theorems on one-dimensional systems which have no direct relevance to fermions. These will be discussed in Sec. II. Section III will contain the proof of our theorem for certain specialized problems in two or more dimensions. We have added an Appendix on an analogous theorem for certain one-dimensional chains of three-dimensional atoms; the proof uses a different technique from that in Sec. I, insomuch as we switch to the delta function (or lattice gas) representation and use second quantization.

As a preliminary, we should like to recall a well-known theorem on the two-fermion problem, proved many years ago.[1] Consider the general two-particle Hamiltonian[2] (in any number of dimensions)

$$H=\mathbf{p}_1^2+\mathbf{p}_2^2+V(\mathbf{r}_1,\mathbf{r}_2), \tag{1}$$

where V is any symmetric potential. That is to say, the particles may interact with each other and/or with an external potential, the only proviso being that no spin- or velocity-dependent forces are present. The boundary conditions can be anything so long as they are homogeneous. Since the total spin S is a good quantum number, the ground state is either $S=0$ or $S=1$. The theorem states that the ground state always has $S=0$, a statement borne out by the hydrogen molecule, for example.

Since V is real (hence the necessity for excluding velocity-dependent forces) the eigenfunctions of H are real. An eigenstate ${}_M{}^S\Psi$ with $S=0$ must be of the form[3]

$${}_0{}^0\Psi=\Phi_{S_y}(\mathbf{r}_1,\mathbf{r}_2)[(+-)-(-+)], \tag{2}$$

where Φ_{S_y} is a symmetric real function and where we have used an obvious notation for the spin part of the wave function. Alternatively, a state with $S=1$ (and $M=1$, for example) must be of the form

$${}_1{}^1\Psi=\Phi_A(\mathbf{r}_1,\mathbf{r}_2)[(++)], \tag{3}$$

where Φ_A is antisymmetric. In both cases the symmetry property of Φ is determined by the Pauli principle which states that ${}_M{}^S\Psi$ must be antisymmetric.

Now if the ground-state wave function were $S=1$, consider the trial function obtained by taking the absolute value of Φ_A,

$${}_0{}^0\Psi\equiv|\Phi_A|[(+-)-(-+)], \tag{4}$$

which has $S=0$ and satisfies the Pauli principle. Φ_A is the spatial part of the $S=1$ ground-state function. It is readily verified that the variational energy of ${}_0{}^0\Psi$ is the same as that of the supposed ground state, ${}_1{}^1\Psi$ (we shall return to a proof of this in Sec. I). Thus, by

[1] The authors believe this theorem is due to E. P. Wigner.

[2] $\hbar^2/2m=1$.

[3] We shall use the notation ${}_M{}^S\psi$ for a function with a definite S and M value; ${}^S\psi$ if it has only a definite S value; and ${}_M\psi$ if it has only a definite M value.

reductio ad absurdum, it follows that there is always an $S=0$ eigenfunction having an energy at least as low as the lowest $S=1$ function. In fact, as we shall show later, the trial function given above cannot be an eigenfunction unless V is pathologic (e.g., a repulsive core in one dimension). Thus, if $E(S)$ denotes the lowest energy belonging to a given S value, $E(0)<E(1)$ for two particles.

This paper is an extension of the two-particle theorem to an arbitrary number of particles. We are able to do it completely for one dimension, and in certain cases for higher dimensions. The general result is $E(S)\leq E(S+1)$.

I. THE ONE-DIMENSIONAL SYSTEM

We start with the general Hamiltonian[2]

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+V(x_1,\cdots,x_N), \tag{5}$$

where V is real and symmetric in the N variables $x_1,\cdots,x_N$. Otherwise, it is completely arbitrary. The boundary conditions may be any of the following:

(i) If the particles are in a "box" (i.e., $0\leq x_i\leq L$), then $\Psi=0$ if any $x_i=0$ or L;

(ii) the same as (i) except that $\partial\Psi/\partial x_i=0$ if any $x_i=0$ or L;

(iii) if $-\infty<x_i<\infty$ or $0<x_i<\infty$, then we restrict ourselves to square integrable (bound state) wave functions, assuming these exist. Periodic boundary conditions are excluded, for they require a slight modification of the theorem and a somewhat lengthier analysis.

Although H does not contain the spins explicitly, every eigenfunction belongs to a definite S value, which may take on any of the values $N/2$, $(N/2)-1$, $\cdots$, 0, or $\frac{1}{2}$. If we denote the lowest or ground-state energy belonging to a given S value by $E(S)$, then the theorem to be proved is

Theorem I. If $S>S'$, *then* $E(S)>E(S')$ *unless* V *is pathologic, in which case* $E(S)\geq E(S')$.

The term pathologic potential will be defined in the sequel.

In order to prove this theorem it is first necessary to characterize the spatial part of a wave function of space and spin. To this end, let ${}_M\Psi$ be a wave function satisfying the Pauli principle and having a definite spin azimuthal quantum number M. (That is, $S_z\,{}_M\Psi=M\,{}_M\Psi$, where $S_z=\sum_{i=1}^{N}S_z^i$.) Then ${}_M\Psi$ may be expanded in the complete set of spin functions having the M value in question. The coefficients of the expansion will be spatial functions. Thus

$${}_M\Psi=\sum_j {}_M\Phi_j(x_1,\cdots,x_N)G_j^M, \tag{6}$$

where G_j^M is a spin function of which a typical one is

$$G_1^M=(\underbrace{--\cdots--}_{p}\underbrace{++\cdots++}_{N-p}),$$

with

$$p=(N/2)-M \tag{8}$$

(i.e., particles $1-p$ have spins down, the rest being up). Since ${}_M\Psi$ is a Pauli function and since the various G_j^M are obtained from each other by a permutation of the spin variables, it follows that the ${}_M\Phi_j$ are related to each other by a permutation of $x_1,\cdots,x_N$. Moreover, the following is easily verified:

(a) If any ${}_M\Phi_j\equiv 0$, then all ${}_M\Phi_j\equiv 0$.

(b) If Ψ is an eigenfunction of H with energy E, then so is each ${}_M\Phi_j$ separately.

(c) ${}_M\Phi_1$ (henceforth to be denoted simply by ${}_M\Phi$) is nonvanishing and is of the form

$${}_M\Phi=\Phi(x_1,\cdots,x_p|\,x_{p+1},\cdots,x_N),\quad p=(N/2)-M, \tag{9}$$

where the notation is meant to imply that Φ is antisymmetric in the variables $x_1,\cdots,x_p$ *and* in the variables $x_{p+1},\cdots,x_N$.

(d) Given any spatial function having the symmetry properties of (9) above, it may be used to generate a nonvanishing Pauli function such as ${}_M\Psi\equiv\sum_p(-)^p\times(p\Phi)(pG_1^M)$, where the summation is over all permutations p of the N particles. If Φ is an eigenfunction of H, then so is ${}_M\Psi$.

The next question to consider is what further condition must we impose on ${}_M\Phi$ in order that ${}_M\Psi$ have a definite S value (i.e., $S^2\,{}_M{}^S\Psi=S(S+1)\,{}_M{}^S\Psi$ and $S_z\,{}_M{}^S\Psi=M\,{}_M{}^S\Psi$). For simplicity, let us take $M\geq 0$ (i.e., $p\leq N/2$), in which case the S value of Ψ in Eq. (6) could be any of $M, M+1,\cdots, N/2$, or a mixture of these. Suppose we wish $S=M$. Then, a necessary and sufficient condition is $S_+\,{}_M{}^M\Psi=0$ where $S_+=\sum_{i=1}^{N}S_+^i$. The operator S_+ acts on the G_j^M functions; acting on G_1^M it generates G_1^{M+1} among others. But other G_j^M's also generate G_1^{M+1} and if one sets equal to zero the coefficient of G_1^{M+1} in $S_+\,{}_M{}^M\Psi$, one finds

(e) A necessary and sufficient condition that ${}_M\Psi$ be ${}_M{}^M\Psi$ is that ${}_M{}^M\Phi$ (the coefficient of G_1^M) be of the form (9) and that the bar cannot be moved to the left. By this is meant that ${}_M{}^M\Phi$ cannot be antisymmetrized with respect to the variables $x_p,\cdots,x_N$. In other words,

$$(1-\sum_{j=p+1}^{N}P_{p,j})\,{}_M{}^M\Phi\equiv 0, \tag{10}$$

where $P_{p,j}$ is the simple transposition permutation of x_p and x_j.

(f) If the bar can be moved to the left once, but not twice, then Ψ is, in general, a mixture of ${}_{M+1}{}_M\Psi$ and ${}_M{}_M\Psi$, and so forth.

(g) If $M>0$, we can always lower the M value of Ψ by $S_-\,{}_M\Psi=\text{const}\,{}_{M-1}\Psi\neq 0$, and hence the bar can always be moved to the right. In other words, if a function is of the form (9), the bar can always be moved to the right if $p<N/2$, but it cannot always be moved to the left. This is a known result of the theory of the

permutation group which we have proved by recourse to the more generally known theory of angular momentum.

(h) Any function satisfying (9) and (10) may be used to generate a nonvanishing ${}_M{}^S\Psi$ as in (d) above. These remarks tell us that the higher the S value of ${}^S\Phi$, the more antisymmetric it must be. For instance, a totally antisymmetric function always belongs to $S=N/2$, but to any $M\leq N/2$.

Now since S_- and S_+ commute with H, $E(S)$ is degenerate with respect to M value; i.e., $H\,{}_M{}^S\Psi = E(S)\,{}_M{}^S\Psi$ implies there exists ${}_j{}^S\Psi$ with the same eigenvalue, where j can take all $2S+1$ values between S and $-S$. We shall therefore prove Theorem I in the following manner: Let $E(M)$ and ${}_M\Psi$ be the lowest eigenvalue and eigenfunction, respectively, of H belonging to a given M value ≥ 0. We shall show that ${}_M\Psi$ is ${}_M{}^M\Psi$ and hence that $E(M)=E(S)$. We shall further show that $E(M)<E(M+1)$ unless V is pathologic. In other words, we shall show that the lowest eigenfunction of H of the form (9) also satisfies Eq. (10).

Let R be the full domain, all $0\leq x_i\leq L$ [assuming we use boundary condition (i) or (ii) for example], and define $R_M\subset R$ by

$$R_M\colon\quad 0\leq x_1\leq\cdots\leq x_p\leq L$$

and

$$0\leq x_{p+1}\leq\cdots\leq x_N\leq L. \tag{11}$$

Consider the Schrödinger equation in R_M;

$$H\varphi=E\varphi, \tag{12}$$

with boundary conditions:

$$\varphi=0 \text{ on the boundary of } R_M. \tag{13}$$

It is well known that the ground-state function φ_0 of Eqs. (12) and (13) satisfies

$$\varphi_0\geq 0 \quad \text{in} \quad R_M. \tag{14}$$

For suppose (14) were not satisfied and consider $\varphi=|\varphi_0|$. Now $\langle\varphi|\varphi\rangle=\langle\varphi_0|\varphi_0\rangle$ and $H\varphi=E\varphi$ everywhere except where φ_0 vanishes, at which points φ is continuous but has discontinuous derivatives. Thus $H\varphi=E\varphi+\delta$ functions, the latter occurring when φ vanishes. Hence

$$\int_{R_M}\varphi(H\varphi)=E\int_{R_M}\varphi\varphi=E\langle\varphi|\varphi\rangle.$$

Therefore φ satisfies the same boundary conditions as φ_0 and has the same variational energy. This implies that among the ground states of (12) and (13) (assuming the possibility of a degeneracy) there is at least one satisfying (14). The following are also true, although the proof is tedious:

(i) If V is bounded, then in fact $\varphi_0\neq 0$ *inside* R_M.

(j) There can be no degeneracy unless $\varphi_0=0$ *inside* R_M.

We can now define the term "pathologic potential." It is a potential with a sufficiently strong infinity to cause φ_0 to vanish *inside* R_M. An infinite repulsive core is an example. Thus there is, in general, no ground-state degeneracy, but even if there is, one of the eigenfunctions satisfies (14).

Let P be a permutation of the variables $x_1,\cdots,x_p$ and Q a permutation of the variables $x_{p+1},\cdots,x_N$, and define $PQ(R_M)$ as the domain defined by the appropriate permutation of the variables in condition (11). All the domains $PQ(R_M)$ are disjoint, except possibly for the boundaries, and together span R. Let φ be any solution to (12) and (13) and define the function Φ everywhere in R by

$$\Phi=(-)^P(-)^Q PQ\varphi \quad \text{in} \quad PQ(R_M). \tag{15}$$

Because of the boundary conditions, (13), it is easily verified that Φ is continuous and has a continuous derivative everywhere in R, and hence satisfies

$$H\Phi=E\Phi \quad \text{in} \quad R. \tag{16}$$

Conversely, any eigenfunction of H in R that satisfies Eq. (9) satisfies (12) and (13) in R_M. Thus if φ_0 is the ground state of (12) and (13), Φ, as defined by (15), is the ground state of H belonging to M.

Now consider

$${}_M{}^M\chi=\mathrm{Det}\begin{vmatrix}1x_1\cdots x_1{}^{p-1}\\ \vdots\quad\ \vdots\\ 1x_p\cdots x_p{}^{p-1}\end{vmatrix}\times\mathrm{Det}\begin{vmatrix}1x_{p+1}\cdots x_{p+1}{}^{N-p-1}\\ \vdots\qquad\ \vdots\\ 1x_N\quad\cdots x_N{}^{N-p-1}\end{vmatrix}$$

$$=\prod_{\substack{j,k=1\\ j>k}}^{p}(x_j-x_k)\times\prod_{\substack{j,k=p+1\\ j>k}}^{N}(x_j-x_k). \tag{17}$$

(Except for a totally symmetric Gaussian factor, this is the solution to the problem of noninteracting one-dimensional electrons in a harmonic oscillator potential.) The function ${}_M{}^M\chi$ clearly satisfies (9), (10), and (14). It is easily verified that if ${}_M{}^S f$ and ${}_M{}^{S'}g$ are any two functions having different S values but the same M value, then

$$\int_R {}_M{}^S f\;{}_M{}^{S'}g=P!(N-P)!\int_{R_M}{}_M{}^S f\;{}_M{}^{S'}g,$$

$$(p=\tfrac{1}{2}N-M) \tag{18}$$

and further the right-hand side of (18) vanishes if $S\neq S'$. Since ${}_M{}^M\chi$ and the ground state of H belonging to M, ${}_M\varphi$, are both non-negative in R_M, Eq. (18) implies that ${}_M\varphi$ is not orthogonal to ${}_M{}^M\chi$ in R. If the ground state of (12) and (13) is nondegenerate, then ${}_M\varphi$ can belong to only one S value and this S value must therefore be $S=M$. If one wants $S=M+1$ or higher, it is necessary to go at least to the first-excited state of (12) and (13). In case of degeneracy, at least one of the ground-state functions belongs to $S=M$.

This completes the proof of Theorem I.

II. GENERALIZATION OF THEOREM I, AND THE "POURING PRINCIPLE"

Thus far we have considered eigenfunctions of H which have the symmetry property (9), the only allowed symmetry class for constructing a Pauli function of space and spin. But there are other symmetry classes with their corresponding eigenfunctions—the totally symmetric function, for example. The latter is a Bose function and plays no role for fermions, unless only two particles are involved.

The most widely known classification of symmetry classes is due to Young; but we shall find it convenient to use a slightly modified version of his scheme.[4] It is well known that every function of 2 variables can be written as the sum of an antisymmetric and a symmetric function which *a fortiori* are orthogonal to each other. Thus,

$$\phi(x_1,x_2)=\tfrac{1}{2}(1+p_{12})\phi+\tfrac{1}{2}(1-p_{12})\phi. \qquad (19)$$

The operator $1-p_{12}$ is said to antisymmetrize ϕ, while the operator $1+p_{12}$ symmetrizes it. If ϕ is a function of $x_1, \cdots, x_N$, the operator $1-p_{12}$ antisymmetrizes it with respect to the variables x_1, x_2; the operator $(1-p_{13}-p_{23})(1-p_{12})$ antisymmetrizes it with respect to x_1, x_2, x_3, and so forth. It is quite possible that ϕ may be antisymmetrized with respect to x_1 and x_2, but not with respect to x_1, x_2, x_3; $(x_1-x_2)x_3$ is an example of such a function.

Now consider a function ϕ of the variables $x_1, \cdots, x_N$ which is of the form

$$\phi(x_1,\cdots|\cdots x_{N-n_1-n_2}|x_{N-n_1-n_2+1},\cdots,x_{N-n_1}| x_{N-n_1+1},\cdots,x_N), \qquad (20)$$

or any of its permutations, by which we mean that it is separately antisymmetric in the n_1 variables $x_{N-n_1+1}, \cdots, x_N$ and in the n_2 variables $x_{N-n_1-n_2+1}, \cdots, x_{N-n_1}$ and so forth, where $n_1 \geq n_2 \geq \cdots$. The bars are to be regarded as unmovable leftwards[5]; e.g., ϕ cannot be antisymmetrized with respect to $x_{N-n_1}, \cdots, x_N$. The function ϕ is said to belong to the symmetry class characterized by the numbers n_1, n_2, etc. For example, a totally symmetric function has N "boxes" with one variable in each, whereas an antisymmetric function has 1 "box" containing all N variables. It is possible to prove the following properties of ϕ:

(a) Any bar may always be moved to the right (i.e., the antisymmetrization procedure which would move the bar to the right gives a nonvanishing result) if the number of variables to the right of the bar is greater than the number to the left.

(b) The largest group of variables with respect to which ϕ may be antisymmetrized is n_1. From among the remainder, the largest group would be n_2, and so forth.

(c) If ϕ and ψ belong to two different symmetry classes, they are orthogonal.

(d) For a function of the form (20), the antisymmetrization operator which moves a bar to the right has as its unique inverse the operator which moves the bar to the left. Therefore, if ψ is obtained from ϕ by moving a bar to the right, it is said to belong to the same class as ϕ.

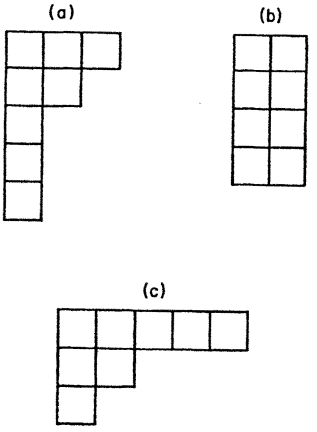

FIG. 1. The tableaux corresponding to several different symmetry classes for eight particles. By the pouring principle $E(a)>E(c)$ and $E(b)>E(c)$, but one cannot say whether (a) or (b) has the lower energy. Note that (c) happens to be the conjugate of (a).

From these remarks we see that by a combination of antisymmetrization and orthogonalization, one can reduce an arbitrary function to a sum of orthogonal functions, each belonging to a different symmetry class. The function in each symmetry class itself is decomposable into a sum of functions of the form (20) and its permutations, although this last decomposition is not unique.

There is a convenient pictorial representation for the symmetry classes called *tableau* illustrated in Fig. 1. One draws a column of n_1 boxes. To the right of it, and starting at the same height, one places a column of n_2 boxes, and so forth. A function of the form (20) is further designated by inserting the appropriate variables in the appropriate column, the order of the variables in any column being immaterial. It will be seen that the lengths of the *rows* decrease from top to bottom; it is therefore possible to define the conjugate to a symmetry class to be the one in which rows are replaced by columns. Thus (a) and (c) in Fig. 1 are conjugate. We shall return to this later, however.

Returning to the problem at hand, it will be appreciated that since H is permutation-invariant, every eigenfunction not only belongs to a definite symmetry class, but is of the form (20). Theorem I, then, tells us about the order of the ground-state energies of functions of the one- and two-column class. Under certain circum-

[4] See, for example, D. E. Rutherford, *Substitutional Analysis* (Edinburgh University Press, Edinburgh, 1948). Young's scheme proceeds by symmetrization, instead of antisymmetrization as used here.

[5] We have departed slightly from the notation in Eq. (9). Formerly the bar was regarded as possibly movable leftwards.

stances it is possible to extend this theorem to more than two-column classes. To do this we need one more concept, which we shall call the "pouring principle."

Definition. If α and β are two different symmetry classes, it is possible to *pour α into β* if the bars in the α function can be moved to the right [subject to (*a*) above] so that one gets a function antisymmetric in the same groups of variables as the β function. More formally, if the α tableau has the columns $n_1 \geq n_2 \geq$, and the β tableau has the columns $n_1' \geq n_2' \geq \cdots$, then we require that $n_1 \geq n_1'$; $(n_1-n_1')+n_2 \geq n_2'$; $(n_1-n_1'+n_2-n_2')+n_3 \geq n_3'$; etc., where any missing columns are to be regarded as having $n=0$. If α can be poured into β, we denote this fact by $\alpha \xrightarrow{p} \beta$.

Thus, in Fig. 1, (a) can be poured into (c) and (b) into (c), but neither (a) nor (b) can be poured into the other. Note that if α can be poured into β, then the conjugate of β can be poured into conjugate of α. We can now state the extension of Theorem I in one dimension.

Theorem II. Let α and β be two symmetry classes and let $E(\alpha)$ and $E(\beta)$ be the respective ground-state energies of eigenfunctions of H in the two classes. If α can be poured in β, then $E(\alpha) > E(\beta)$ unless V is pathologic, in which case $E(\alpha) \geq E(\beta)$.

The proof is exactly the same as for Theorem I. One antisymmetrizes the α function until it matches the bars of the β function (a process which does not change the energy of the α function). Next one defines the fundamental region in analogy with (11) above and shows that the ground-state function in this region is positive, and is therefore not orthogonal to a determinantal function which is positive in this region and is known to belong to the β class.

Corollary: Consider[2]

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}-\sum_{i=1}^{M}\frac{\partial^2}{\partial y_i^2}+V(x_1,\cdots,x_N;\, y_1,\cdots,y_M). \quad (21)$$

If V is symmetric in the x variables, then every eigenfunction belongs to some symmetry class under permutation of these variables. Theorem II obviously is true for this more general problem. If, moreover, V is also separately symmetric in the y variables, although of no particular symmetry under the interchange of an x with a y, then every eigenfunction falls into some symmetry class α in the x variables and some class α' in the y variables. If two functions are characterized by (α,α') and (β,β'), respectively, then $E(\alpha,\alpha') > E(\beta,\beta')$ if α can be poured into β and α' into β'.

III. SEPARATELY SYMMETRIC POTENTIAL IN HIGHER DIMENSIONS

We shall now turn to the proof of the extension of Theorem I to higher dimensions when the potential is separately symmetric. Only two dimensions will be explicitly considered, for the extension to three dimensions is a corollary. The general fermion Hamiltonian is of the form (21) with $M=N$ and V is a symmetric function of the pairs x_1, y_1, etc. A separately symmetric potential is one for which V is, in addition, separately symmetric in the x variables, and in the y variables. The theorem to be proved is:

Theorem III. If V is separately symmetric and if $S > S'$, then $E(S) \geq E(S')$. (Note that Theorem III is not quite so strong as Theorem I, because the equalities can occur without pathologic potentials.)

Before discussing Theorem III, it is necessary to consider the "Kronecker product" of two tableaux. Suppose we have a function of the x's and the y's which is of a definite symmetry class α in the x's and a definite class α' in the y's. Let us consider this function together with all the functions derived from it by permutations, and let us ask if there is some linear combination of these functions which is of a definite symmetry class, β, in the N *pairs* of variables (x_i,y_i). If so, which β classes can be generated and how many independent β functions are there? [By independent β functions we mean functions which cannot be obtained from each other by permutations of the (x_i,y_i) pairs.] This question is analogous to the problem in the theory of angular momentum of combining J_1 and J_2 to give a resultant J. There the answer is given simply by the Clebsch-Gordan theorem: All $J_1+J_2 \geq J \geq |J_1-J_2|$ may be produced once and only once. Unfortunately, there is no such simple rule for tableaux except in two special cases: when β is symmetric, or antisymmetric (i.e., one row, or one column).

Lemma I. To generate a totally antisymmetric function in the pairs $x_i y_i$, it is required that the x and y tableaux α and α' be conjugates. (To generate a totally symmetric function in the pairs, the x tableau must be the same as the y tableau.)

This is a well-known result from the theory of permutation groups.[4]

As we saw in Sec. I, the spatial part of a Pauli (antisymmetric) function of definite S must be of the two-column type, where $n_1=(N/2)+S$ and $n_2=(N/2)-S$. By Lemma I we are led to believe that spin functions of a given S are of the conjugate two-row type. This is indeed the case. There are $\binom{N}{p}$ different G_M functions, and these will be seen to generate all two-row tableaux in which the first row is $(N/2)+M$ or longer. Because the ${}_M\varphi_j$ in Eq. (6) are all derivable from each other, they will not all be linearly independent. The $G_j{}^M$'s therefore appear only in certain definite linear combinations; if φ is of the two-column type, these linear combinations can be shown to be of the conjugate two-row type.

Any Pauli eigenfunction of H of definite S value is thus seen to be the triple Kronecker product of a function belonging to the α and α' class in the x and y variables, respectively, and of a two-row function of the spin variables. The resultant must be a one-column function in the triplets (x_i,y_i,s_i), where s_i is the spin variable. The

problem can be viewed in two ways: a Kronecker product of α and α' must be of the appropriate two-column type; or a Kronecker product of α and the two-row spin function must be conjugate to α'.

To prove Theorem III, we take the latter view. Let α and α' be the tableaux of the spatial function, giving the lowest energy for a given S value and suppose α' is (c) of Fig. 1, so that the (x_i,s_i) class, which we shall denote by β, is (a) of Fig. 1. A typical representative, χ, would have each of the pairs (x_i,s_i) in some box of the (a) tableau and each of the y_i in some box of the (c) tableau. Suppose x has $(x_1,s_1), \cdots, (x_5,s_5)$ in the first column, (x_6,s_6) and (x_7,s_7) in the second, and (x_8,s_8) in the third. It will be seen that χ may be regarded as a five-particle one-dimensional Pauli function in the first five pairs, or as a two-particle Pauli function in the next two pairs.

Now, to prove Theorem III we need the following lemma:

Lemma II. Let χ be an eigenfunction with the following properties: (1) it is of the α and α' symmetry classes in the x and y variables, respectively, and is in fact formed from the lowest eigenfunction of H having these classes; (2) in the (x,s) pairs, it is antisymmetric in the same sets of variables as a function of class β, the conjugate of α', but it is not necessarily itself of the class β; (3) considered as a function of each of the sets of (x,s) pairs in which it is antisymmetric, it has a definite S value (i.e., each column has a definite S value). These S values we shall call $S_1, S_2, \cdots$. Let S be any total S value for all the particles which can be compounded from $S_1, S_2, \cdots$ by the usual Clebsch-Gordan rule. Then $E(S) \leq E(\alpha,\alpha')$.

Proof. By applying the appropriate S_+ and S_- operators of each column the appropriate number of times to χ, we can generate functions having all possible M values in each column and which still have the same energy as χ. These functions are then to be added together with the appropriate coefficients to generate a new function, ${}^S\chi \neq 0$ having the required total S value. ${}^S\chi$ has the same energy as χ. Since the total S^2 operator commutes with all permutations, ${}^S\chi$ may be written as the sum of functions belonging to definite symmetry classes and all having the given S value. One of these tableaux may be β itself, in which case the lemma is proved. If not, then since ${}^S\chi$ is already antisymmetric in the same sets of variables as the β tableau, at least one of the component tableaux, say γ, must be such that $\gamma \xrightarrow{P} \beta$. To make a Pauli function out of this component we should need a function whose y class is γ^+, the conjugate of γ. But γ^+ satisfies $\alpha' \xrightarrow{P} \gamma^+$, and therefore $E(\alpha,\gamma^+) \leq E(\alpha,\alpha')$. Thus, if we carry out the same procedure again with the ground-state function of the (α,γ^+) class, we shall be able to construct a Pauli function having the S value in question and with an energy lower than $E(\alpha,\alpha')$.

Corollary. The ground-state function of a given S value has the properties of χ above, and, moreover, belongs to the symmetry class β in the (x,s) variables.

Proof. If not, then by the procedure of the above proof, we should either be able to lower the energy by changing the y tableau, or else we should end up with the function ${}^S\chi$ having the properties stated in the corollary.

Now we consider the proof of Theorem III. The lowest eigenfunction having a given $S \neq 0$ value is the sum of permutations of a function ${}^S\chi$ having the properties stated in the corollary and therefore has the S values S_1, S_2, etc., in each column of β, the (x,s) tableau. There are three cases to be considered:

(1) If S is not the minimum that can be compounded of S_1, S_2, etc., then we can construct a function of spin $S-1$ and with at least as low an energy.

(2) If S_1, S_2, etc., are already the lowest possible (i.e., either 0 or $\frac{1}{2}$) then (1) above is transparently true.

(3) If S is indeed the minimum of $S_1 \oplus S_2 \oplus$, etc., then lowering some one of these S_i values, say S_1, would permit us to create a function of total S equal to $S-1$. But there does exist a function having a lower energy than ${}^S\chi$ and having the properties of χ listed in Lemma II, except that the first column has the value S_1-1. To see this, we regard the function having the α tableau in the x's as being the sum of functions each belonging to definite symmetry classes in each of the groups of x variables appearing in each column of β. One of these sets of tableaux must be the respective conjugates of S_1, S_2, etc. Looking at χ from this point of view, it is clear from the results of Secs. I and II that we can lower one or more of the S_i at will and at the same time lower the energy.

This completes the proof of Theorem III for two dimensions; the extension to higher dimensions is obvious: We simply treat the s_i, z_i pairs in the same manner as the spins above. Let us remark, however, on the reason for the lack of strict inequality as we had in Theorem I. Suppose the lowest function of $S=1$ had an (x,s) tableau such as (a) in Fig. 1 with $S_1=S_3=\frac{1}{2}$ and $S_2=0$. Since each column already has its lowest possible S value, the only way in which $S=0$ could have a *lower* energy is by having an (x,s) tableau containing only columns of even length, such as (b) of Fig. 1, with $S=0$ in each. But it is not possible to prove that such a function has, in fact, a lower energy, and therefore it is possible for the ground state as well as for excited states to have a degeneracy in more than one dimension. (This degeneracy can be estimated never to exceed $N^{\frac{1}{2}}$, in three dimensions. It is therefore not an extensive property of the system.)

IV. ON THEORIES OF FERROMAGNETISM

Although we could extend them to other particles obeying various statistics, the results of this paper apply most directly to the problem of interacting

electrons, and as such have some bearing on the theory of ferromagnetism.

It is well known that ferromagnetism must be a consequence of the electronic interactions, for a noninteracting electron system always obeys the theorem $E(S)\leq E(S+1)$, regardless of the external potential. This is antiferromagnetism, or at most, paramagnetism. Ferromagnetism is assumed to occur when the ground state belongs to a nonvanishing S whose magnitude is proportional to the size of the system. It is also well known that the direct magnetic spin-spin forces are negligibly weak, so that the spatial forces in conjunction with the Pauli principle are held to be responsible for the phenomenon.

The simplest realistic problem which offers some hope of being soluble is the linear chain of three-dimensional atoms. The atomic states are supposed known when the atoms are infinitely far apart, and the problem is to find the new configurations when overlap becomes important. Peierls[6] considers this very problem in the chapter on ferromagnetism in his book. The approximation which he makes is that there is only one orbital state per atom, and he concludes that the electronic interactions can lead to ferromagnetism. However, recent and more realistic calculations[7-9] on such chains have proved the contrary to be true. Also in Sec. I we showed that under no circumstances can a one-dimensional electron system be ferromagnetic with only space-dependent forces; this includes the special case of a chain of one-dimensional "atoms." In the Appendix we also treat a model applicable to an idealized chain of three-dimensional atoms, with similar results. It therefore seems that a linear chain can be magnetic only if the individual atoms have orbital degeneracy, that is, if the single atom displays a magnetic or truly three-dimensional character; but it is not known whether this is a *sufficient* condition for ferromagnetism to occur in a linear system.

Our theorem has no relevance to atomic magnetism *per se* (Hund's rule) because it does not apply to the central force problem in three dimensions. But if we consider ferromagnetism to be an extensive property of a solid, the theorem does have some relevance. For we shall show that it is not merely sufficient to have (i) a band structure, (ii) strong repulsive interactions, and (iii) three dimensions, to produce ferromagnetism. We shall base ourselves on the results of Sec. III.

Suppose, for example, that highly magnetized states of a noninteracting set of electrons lie rather close in energy to the $S=0$ ground state. If one introduces a repulsive interaction potential into the problem, and treats this by lowest-order perturbation theory, certain terms called the "exchange integral" will favor the magnetized states. To lowest order, one may find that the magnetized states have crossed the $S=0$ state, and the interacting system is supposed to become ferromagnetic. But this conclusion would be fallacious if the effect were cancelled by second-order or higher-order terms in the perturbation series (or if the perturbation expansion did not converge). Indeed, we now give an example based on the previous section, which is a case in point. Consider, for example, the unperturbed Hamiltonian to be

$$H_0=\sum p_i^2+\sum_i [V(x_i)+V(y_i)+V(z_i)]. \quad (22)$$

Let $V(x)$ be a periodic potential so that one-electron eigenfunctions are Bloch functions. The potential can be chosen such that the bands display the usual degeneracies and other features of motion in a three-dimensional cubic lattice.

If now we introduce an interaction, say

$$H_I=g^2\sum_{ij}\left(\frac{1}{|x_i-x_j|+d}+\frac{1}{|y_i-y_j|+d}+\frac{1}{|z_i-z_j|+d}\right), \quad (23)$$

or some other repulsive, separately symmetric interaction, the total Hamiltonian H_0+H_I is still subject to our theorem and is *not* ferromagnetic. (The theorem does not exclude paramagnetism, however, for the ground state might be degenerate with states of nonvanishing spin angular momentum.) But what are the conclusions we would reach if we were to apply first-order perturbation theory to H_I? This amounts to calculating the expectation value of H_0+H_I using the Slater determinants appropriate to the unperturbed problem. The unperturbed functions with the most spatial nodes are better, variationally speaking, than those with fewer nodes for *sufficiently large* g^2, and we might be led to conclude that there exist some values of S such that $E(S)<E(0)$, which is erroneous. It is therefore clear that we cannot always trust perturbation theory to properly order the levels, for when it is carried out only to finite order, it might be more accurate for some values of S than for others, depending on the particular features of the problem. The same can be said of variational calculations.

A notorious example of the above is the low-density electron gas with Coulomb interactions which is in a background of compensating positive charge. The expectation value of the Hamiltonian using the unperturbed plane-wave states is lower for the ferromagnetic configuration than for the nonferromagnetic ones, at sufficiently low density. But perturbation theory diverges for this problem,[10] and this ferromagnetism is indeed fictitious. A recent and accurate calculation[11] by

[6] R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, New York, 1955).
[7] R. K. Nesbet, Phys. Rev. 122, 1497 (1961).
[8] L. F. Mattheiss, Phys. Rev. 123, 1209 (1961).
[9] David I. Paul, Phys. Rev. 118, 92 (1960), and Phys. Rev. 120, 463 (1960).
[10] M. Gell-Mann and K. A. Brueckner, Phys. Rev. 106, 364 (1957).
[11] W. J. Carr, Jr., Phys. Rev. 122, 1437 (1961).

Carr leads that author to conclude that at all but the lowest densities the electronic spins are *antiferromagnetically* aligned.

In concluding, we should recall that our theorem is not valid if there are explicitly spin-dependent forces, or velocity-dependent forces. In the latter case, the eigenfunctions are not real and our method of proof does not apply. Nor does it apply to the Coulomb potential which governs real electrons. But it does serve as a warning that the criterion for ferromagnetism must be rather detailed, and not so broad as to violate the results of this investigation.

We have also found it possible to order many of the energy levels of the Heisenberg Hamiltonian $\sum K_{ij}\mathbf{S}_i\cdot\mathbf{S}_j$ (where the S_i are spins on a lattice in one, two, or three dimensions), by analogy with the calculation in the Appendix. These results will be reported in a subsequent publication.

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APPENDIX. ONE-DIMENSIONAL LATTICE GAS

We are interested in a theorem analogous to the one in the text, for a chain of *three*-dimensional atoms. This problem cannot be solved in all generality, therefore we are led to consider the following tractable model.

(a) We use a truncated Hamiltonian such that only valence electrons are mobile.

(b) Each atom in the linear chain has only one valence state (capable of double occupancy, however, because of spin degeneracy).

(c) The atoms are at a distance d from their nearest neighbors. This distance is such that only nearest-neighbor overlap is important.

(d) The matrix element for a one-electron hop from site j to $j\pm1$ is K, a constant. Two-electron hops and exchange effects are neglected. This is equivalent to

(e) assuming that aside from the "hopping" matrix elements the Hamiltonian is diagonal, with an energy calculable by specifying which atoms have empty valence states, which have singly occupied valence state, and which have doubly occupied valence states. These assumptions lead directly to Eq. (A4).

Our model reduces, in a certain limit, to the one-dimensional problem of Sec. I. The Appendix provides therefore an alternate proof for Theorem I.

To see this, let us consider one-dimensional space as consisting of discrete points labeled $i=1, 2, \cdots, N$, separated by a distance d. The length of the chain is therefore Nd. Next, introduce the second-quantized Fermi operators c_{is} and $c_{is}^\dagger$, where $s=$"up" or "down" according to the spin coordinate, and

$$[c_{is},c_{js'}]_+=0,\quad [c_{is}^\dagger,c_{js'}]_+=\delta_{ij}\delta_{ss'}. \tag{A1}$$

Now consider the Hamiltonian

$$H=-K\sum_{i,s}(c_{i+1,s}^\dagger c_{is}+c_{i-1,s}^\dagger c_{is}-2c_{is}^\dagger c_{is}) + \sum_{i,j,s,s'} V(|i-j|)c_{is}^\dagger c_{is}c_{js'}^\dagger c_{js'}. \tag{A2}$$

If we transform to running waves,

$$H\rightarrow 2K\sum(1-\cos kd)c_{ks}^\dagger c_{ks} +\sum V_q c_{k+qs}^\dagger c_{ks}c_{k'-qs'}^\dagger c_{k's'}, \tag{A.3}$$

where V_q is the Fourier transform of $V(|i-j|)$. In the limit $K^{-\frac{1}{2}}=d=N^{-1}=0$ this reduces to the problem of a one-dimensional electron gas with two-body forces. The Hamiltonian (A2) is a special case of the problem we shall now consider,

$$H=-K\sum_{i,s}(c_{i+1,s}^\dagger c_{is}+\text{H.c.})+V(\cdots n_j\cdots), \tag{A4}$$

where V is an arbitrary symmetric function of the operators $n_j\equiv(c_{j\uparrow}^\dagger c_{j\uparrow}+c_{j\downarrow}^\dagger c_{j\downarrow})$. This Hamiltonian satisfies (a)–(e), is identical with the general Hamiltonian of Sec. I in the limit $K^{-\frac{1}{2}}=d=0$, and can be shown to commute with the spin operators which, in our new representation, are

$$S_z=\tfrac{1}{2}\sum_i(c_{i\uparrow}^\dagger c_{i\uparrow}-c_{i\downarrow}^\dagger c_{i\downarrow}),\quad S_y=\tfrac{1}{2}i\sum(c_{i\uparrow}^\dagger c_{i\downarrow}-c_{i\downarrow}^\dagger c_{i\uparrow}),$$

and

$$S_x=\tfrac{1}{2}\sum(c_{i\uparrow}^\dagger c_{i\downarrow}+\text{H.c.}). \tag{A5}$$

The problem is soluble because there exists a transformation to Pauli (pseudo-spin) variables, in which the Schrödinger equation can be reduced to a series of algebraic equations. We define the Pauli operators as follows:

$$\begin{aligned} b_{i\downarrow}&\equiv c_{i\downarrow}\exp\{\pi i\sum_{j=1}^{i-1}c_{j\downarrow}^\dagger c_{j\downarrow}\},\\ b_{i\uparrow}&\equiv c_{i\uparrow}\exp\{\pi i[\sum_{j=1}^{N}c_{j\downarrow}^\dagger c_{j\downarrow}+\sum_{j=1}^{i-1}c_{j\uparrow}^\dagger c_{j\uparrow}]\},\end{aligned} \tag{A6}$$

The $b_i^\dagger$'s are given by the Hermitean conjugates of these defining equations. All Pauli operators *commute except* b_{is} and $b_{is}^\dagger$, (for all i and s), which anticommute:

$$b_{is}^\dagger b_{is}+b_{is}b_{is}^\dagger=1. \tag{A7}$$

In terms of these new operators,

$$H=-K\sum(b_{i+1,s}^\dagger b_{is}+\text{H.c.})+V(\cdots n_j\cdots), \tag{A8}$$

where $n_j=b_{j\uparrow}^\dagger b_{j\uparrow}+b_{j\downarrow}^\dagger b_{j\downarrow}$. The Hamiltonian remains simple under this transformation only for this very special case of a linear chain, and nearest-neighbor hops. We now assume $K>0$. Otherwise, K can be made positive by a trivial canonical transformation.

Also, for the moment, let us pretend that the number of electrons is even, and is $2p$. Obviously, p cannot exceed N, the number of sites, as each site can accommodate two electrons at most.

Ground State in $M=0$ Subspace

States of all allowed spin angular momentum can be rotated into the $M=0$ subspace with no change in energy. The ground state here is therefore the ground state of the Hamiltonian. The configurations which form a complete set in this subspace have p electrons with spin up and p with spin down. (A configuration specifies which sites are vacant or occupied); for example, if $p=1$ and $N=2$, the complete set of $M=0$ configurations is

$$\phi_1=b_{1\uparrow}{}^{\dagger}b_{1\downarrow}{}^{\dagger}|0\rangle, \qquad \phi_2=b_{2\uparrow}{}^{\dagger}b_{2\downarrow}{}^{\dagger}|0\rangle,$$
$$\phi_3=b_{1\uparrow}{}^{\dagger}b_{2\downarrow}{}^{\dagger}|0\rangle, \quad \text{and} \quad \phi_4=b_{1\downarrow}{}^{\dagger}b_{2\uparrow}{}^{\dagger}|0\rangle.$$

The Pauli operators for different particles commute, and therefore, the configurations can all be defined to have the same sign for arbitrary ordering of the operators. The number of distinct configurations is $t\equiv\binom{N}{p}^2$, and we shall label them ϕ_α, where $\alpha=1, 2, \cdots, t$.

Let the ground-state function be

$$\psi_0=\sum f^\alpha\phi_\alpha, \tag{A9}$$

with energy E_0 and real amplitudes f^α. If we denote the eigenvalues of V by V_α,

$$V\phi_\alpha=V_\alpha\phi_\alpha, \quad |V_\alpha|<\infty, \tag{A10}$$

then Schrödinger's equation can be expressed in terms of the amplitudes as

$$-K\sum_{\beta(\alpha)} f^{\beta(\alpha)}=(E_0-V_\alpha)f^\alpha. \tag{A11}$$

The index $\beta(\alpha)$ runs over those configurations for which

$$\langle\beta(\alpha)|H-V|\alpha\rangle\neq 0. \tag{A12}$$

We parenthetically observe that a variational function,

$$\psi=\sum g^\alpha\phi_\alpha, \tag{A13}$$

has variational energy W,

$$W=\frac{-K\sum\sum g^\alpha g^{\beta(\alpha)}+\sum V_\alpha(g^\alpha)^2}{\sum(g^\alpha)^2}\geq E_0. \tag{A14}$$

Clearly, all nonzero amplitudes f^α can be chosen positive in the ground state. For if they oscillate in sign, define a trial function by $g^\alpha\equiv|f^\alpha|$. Then by inspection of (A14), $W\leq E_0$. This is a contradiction unless

$$\psi'\equiv\sum|f^\alpha|\phi_\alpha,$$

is also a ground-state eigenfunction. Therefore,

$$-K\sum_{\beta(\alpha)}|f^{\beta(\alpha)}|=(E_0-V_\alpha)|f^\alpha|. \tag{A15}$$

If any $f^\alpha=0$, then by Eq. (A15) all $f^{\beta(\alpha)}$ also vanish. Since by repeated application of H to any given state, all other states are eventually reached, we can conclude that *all* f^α vanish if some one f^α vanishes. Therefore

$$f^\alpha\neq 0 \text{ for all } \alpha. \tag{A16}$$

(We note that $E_0-V_\alpha<0$ for all α, since the ground-state energy must lie lower than the most favorable potential energy.)

Equations (A11) and (A15) are *incompatible unless* all f^α have the same sign, for if we combine them, we obtain

$$\sum|f^{\beta(\alpha)}|=|\sum f^{\beta(\alpha)}|, \text{ for all } \alpha. \tag{A17}$$

Hence $\psi'=\pm\psi_0$. That the ground state is nondegenerate follows from the observation that all other eigenfunctions of H must be orthogonal to ψ_0 and therefore must have a change of sign, and therefore cannot obey Eq. (A17).

The spin of ψ_0 is found by noting that ψ_0 is *not* orthogonal to the ground state for $V=0$, because they both contain all configurations of Pauli operators with no changes of sign in the amplitudes. The ground state for $V=0$ can be found by inspection of (A3), and belongs to $S=0$. Therefore, the ground state belongs to $S=0$ in general.

Ground State for $M>0$

By a similar procedure, the ground state in any $M>0$ subspace is found to belong to $S=M$. Since each such subspace contains all states of $S\geq M$, this automatically orders the ground states belonging to the various values of S, whether the number of electrons is even or odd. Denoting by $E(S)$ the lowest energy belonging to total spin S, we have therefore proved the following:

Theorem. $E(S+1)>E(S)$.

Note that the restrictions (a)–(e) preclude "double hops," which is related to so-called "exchange." It is therefore reasonable to assume that if ferromagnetism is possible in a linear chain of the sort we have considered, that these neglected exchange matrix elements would be responsible. However, very recent and accurate calculations[7–9] have shown this exchange mechanism to be rather weak. Nesbet[7] finds that the direct "exchange is small compared with the sum of the various antiferromagnetic effects." Mattheiss[8] finds that the true energy levels of such a chain are accurately approximated by the states of the Heisenberg antiferromagnet with nearest-neighbor interactions. Finally, Paul[9] also concludes that linear chains of atoms in s states are nonferromagnetic. It would be interesting to investigate whether an orbital degeneracy on each atom could lead to ferromagnetism for the linear chain in the same way as it appears to be responsible for the magnetic moment of the O_2 molecule.

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Ordering Energy Levels of Interacting Spin Systems

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The total spin S is a good quantum number in problems of interacting spins. We have shown that for rather general antiferromagnetic or ferrimagnetic Hamiltonians, which need not exhibit translational invariance, the lowest energy eigenvalue for each value of S [denoted $E(S)$] is ordered in a natural way. In antiferromagnetism, $E(S+1) > E(S)$ for $S \geq 0$. In ferrimagnetism, $E(S+1) > E(S)$ for $S \geq \mathfrak{s}$, and in addition the ground state belongs to $S \leq \mathfrak{s}$. $\mathfrak{s}$ is defined as follows: Let the maximum spin of the A sublattice be S_A and of the B sublattice S_B; then $\mathfrak{s} \equiv |S_A - S_B|$. Antiferromagnetism is treated as the special case of $\mathfrak{s} = 0$. We also briefly discuss the structure of the lowest eigenfunctions in an external magnetic field.

INTRODUCTION

THE general Heisenberg Hamiltonian for interacting spins on a lattice (in any number of dimensions) is

$$H = 2 \sum J_{ij} S_i \cdot S_j. \tag{1}$$

This describes theories of ferromagnetism, ferrimagnetism, and antiferromagnetism, depending on the geometry of the lattice, the structure of the symmetric matrix J_{ij}, and the magnitude of the intrinsic spins (which may vary from site to site). In fact, it is conceivable that these factors be such that the spin system displays a mixture of the three magnetic properties. But we shall restrict the discussion to *ferrimagnetic* arrays, of which a special case is *antiferromagnetism*.

We consider only those arrays for which an A and a B sublattice can be defined. The definition of these two sublattices is circular, and perhaps not unique, for the only requirement in defining them is that there exist a constant $g^2 \geq 0$ such that for all sites $i(A)$ on one sublattice and $i(B)$ on the other,

$$J_{i(A),i(A)} \leq g^2, \qquad J_{i(B),i(B)} \leq g^2, \qquad \text{and} \quad J_{i(A),i(B)} \geq g^2. \tag{2}$$

In general, there might be several ways to decompose the lattice in such a way that (2) is obeyed, or there may be none. In the latter case, the system is not necessarily ferromagnetic, and only explicit solutions will reveal its properties. But if (2) is obeyed, we shall show that one is definitely dealing with ferrimagnetism or antiferromagnetism. Note that the number of sites in each sublattice and the magnitude of the intrinsic spin on each site is irrevalent, so that only the topology of the lattice and the structure of J_{ij} counts. Note also that for $g = 0$, and the A sublattice consisting of the nearest neighbors to the sites on (i.e., intermeshing with) the B sublattice, the requirement (2) gives a tendency for nearest neighbors to align antiparallel and next-nearest neighbors to align parallel, and therefore reduces to the usual definition of ferrimagnetism (when the spins are of unequal magnitude) and of antiferromagnetism (when all spins are equal).

The intrinsic spin of an electron is 1/2, but we may be dealing with various species of magnetized atoms or nuclei, so let the intrinsic spin angular momentum on each site be s_i. The maximum possible spin S_A on the A sublattice is therefore

$$S_A \equiv \sum_{i(A)} s_{i(A)}, \tag{3a}$$

and on the B sublattice

$$S_B \equiv \sum_{i(B)} s_{i(B)}. \tag{3b}$$

Defining

$$\mathfrak{s} \equiv |S_A - S_B|, \tag{3c}$$

we shall prove that the ground state of H belongs *at most* to total spin $S = \mathfrak{s}$. Moreover, if we denote by $E(S)$ the lowest energy eigenvalue belonging to total spin S, then we shall also prove

$$E(S+1) > E(S) \quad \text{for all} \quad S \geq \mathfrak{s}, \tag{4}$$

and

$$E(S) > E(\mathfrak{s}) \quad \text{for} \quad S < \mathfrak{s} \quad \text{and} \quad g^2 = 0.$$

(Antiferromagnetism is when $\mathfrak{s} = 0$, and the ground state belongs to total spin zero.) This can be regarded *either* as a theorem in ferri- or antiferromagnetism, *or* as a proof that the conditions in Eq. (2) and above eliminate the possibility of ferromagnetism (insofar as it costs energy to raise the total spin value over and above its ground-state value, and that this ground-state value is far from the maximum per-

With D.C. Mattis in J. Math. Phys. 3, 749–751 (1962)

missible value of $S_A + S_B$). It also indicates that a large class of apparently different Hamiltonians (1) have really a similar structure, as summarized in Eq. (4), and in the properties of the corresponding eigenfunctions which we shall find below.

W. Marshall was the first to show[1] that the ground state of an antiferromagnet is a singlet; Elsewhere,[2] we have commented on and strengthened his proof. In the present work, we succeed in removing the requirement of translational invariance, and also apply the method to identify the excited states. The M-subspace arguments presented here were previously found useful in the classification of the states of an electron system, and have been used to disprove the possibility of ferromagnetism in linear chains of atoms in s states.[3]

We shall now restrict the discussion to the special case $g^2 = 0$, until the end of the proof.

M SUBSPACES

With the help of the total spin operator

$$\mathbf{S} \equiv \sum \mathbf{s}_i$$

we can construct two operators which commute with each other and with H, namely, $\mathbf{S}^2$ and $\mathbf{S}_z$, which possess eigenvalues $S(S+1)$ and M, respectively. It is known from the theory of angular momentum that $S \geq |M|$. From the rotational invariance of the Hamiltonian we infer the $(2S+1)$-fold degeneracy of each energy level belonging to S, one degenerate level for each value of M in the range $-S \leq M \leq S$. It therefore follows that every energy eigenvalue has a corresponding eigenfunction (representative) in the $M = 0$ subspace of eigenfunctions; that every energy level except those belonging to $S = 0$ has a representative in the $M = 1$ subspace; similarly for all except $S = 0$ and $S = 1$ in the $M = 2$ subspace, and so forth. The theorem, Eq. (4), will be proved if we can show that the lowest energy in an M subspace belongs to $S = M$, for spin $S + 1$ also has a representative in that subspace and therefore $E(S) < E(S+1)$. If the ground state belongs to $S = S_0$ (we still have to prove that $S_0 \leq \mathfrak{s}$), we need only consider the subspaces of $|M| \geq S_0$, for the ground states of the remaining subspaces will always belong to S_0.

The mechanics of the proof are this: The ground state of H in an M subspace is *not* orthogonal to the ground state of a soluble Hamiltonian in the same subspace, and the latter is *known* to belong to $S = M$ for $M \geq \mathfrak{s}$; therefore, so does the former. Now let us go into more detail.

PROOF

In an M subspace, choose the basis set to consist of all distinct eigenfunctions of the $\mathbf{s}_i^z$ compatible with eigenvalue M. We denote each configuration in the set by ϕ_a, where a is an index which runs over all members of the set. Shortly, we shall specify a convenient choice of phase for each configuration. But first, perform a canonical transformation on H by letting

$$\mathbf{S}_{i(A)}^z \to -\mathbf{S}_{i(A)}^z, \qquad \mathbf{S}_{i(A)}^y \to -\mathbf{S}_{i(A)}^y,$$
$$\mathbf{S}_{i(A)}^x \to +\mathbf{S}_{i(A)}^x \tag{5}$$

but leaving the spins on the B-sublattice invariant. In the *new* language, the Hamiltonian can be written as $H_0 + H_1$, where the diagonal part is

$$H_0 = 2 \sum J_{ij} \mathbf{S}_i^z \mathbf{S}_j^z, \tag{6}$$

and the nondiagonal part is

$$H_1 = -\{\sum |J_{ij}| \, S_i^+ S_j^- + \text{H.c.}\}. \tag{7}$$

We recall that g^2 of Eq. (2) is zero: the generalization for $g^2 > 0$ comes below.

In a given state ϕ_a, S_i^z has eigenvalue m_i. Choose the phase of ϕ_a in the following manner:

$$\phi_a = C(S_1^+)^{S_1+m_1}(S_2^+)^{S_2+m_2} \cdots (S_N^+)^{S_N+m_N}\chi, \tag{8}$$

where χ is the state in which $m_i = -S_i$, and C is a positive normalization constant. With this definition in mind, it is clear that if we define $K_{\beta a}$ to be

$$K_{\beta a} = \langle \phi_\beta \, | H_1 | \, \phi_a \rangle, \tag{9}$$

then

$$K_{\beta a} \leq 0, \quad \text{or equivalently,} \quad K_{\beta a} = -|K_{\beta a}|. \tag{10}$$

The ground state in the M subspace is denoted ψ, belongs to the ground-state energy E_M, and can be expanded in our complete set in terms of the amplitudes f_a,

$$\psi = \sum f_a \phi_a. \tag{11}$$

Since H_0 is diagonal, denote its eigenvalues by e_a,

$$H_0 \phi_a = e_a \phi_a, \tag{12}$$

and therefore the Schrödinger equation reads

$$-\sum_\beta |K_{\beta a}| \cdot f_\beta + e_a f_a = E_M f_a. \tag{13}$$

The variational energy of any trial function exceeds E_M, unless it is also a ground-state eigenfunction.

[1] W. Marshall, Proc. Roy. Soc. (London) **A232**, 48 (1955).
[2] E. Lieb, T. Schultz, D. Mattis, Ann. Phys. **16**, 407 (1961), particularly Appendix B.
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But

$$\psi' = \sum |f_\alpha| \phi_\alpha \tag{14}$$

is a trial function with variational energy E_M, and therefore

$$-\sum |K_{\beta\alpha}| |f_\beta| + e_\alpha |f_\alpha| = E_M |f_\alpha|. \tag{15}$$

Moreover,

$$e_\alpha - E_M > 0, \quad \text{for all} \quad \alpha \tag{16}$$

(otherwise, some *one* ϕ_α would be the ground state, which is in general impossible.) Therefore, taking the absolute value of $(e_\alpha - E_M)f_\alpha$ as given be Eq. (11) and combining with Eq. (15), we obtain

$$|(\sum |K_{\beta\alpha}| f_\beta)| = \sum |K_{\beta\alpha}| |f_\beta|. \tag{17}$$

This is a contradiction unless

$$f_\beta \geq 0 \quad \text{for all} \quad \beta. \tag{18}$$

In general, we have a slightly stronger result,

$$f_\beta > 0, \quad \text{for all} \quad \beta. \tag{19}$$

For, if some f_α vaaished, then Eq. (15) would read:

$$\sum K_{\beta\alpha} |f_\beta| = 0,$$

and by succeeding applications of the Hamiltonian, one could establish that *all* the amplitudes vanished, unless the Hamiltonian splits into sets of noninteracting spins in which case only the weaker result (18) holds. Therefore, in general, all amplitudes are positive and nonvanishing, and hence E_M in nondegenerate. This last statement follows from the impossibility of constructing states orthogonal to ψ without some changes of sign, and consequent violation of the ground-state property (19).

Next consider the special Hamiltonian where $J_{i(A)j(A)} = J_{i(B)j(B)} = 0$ and $J_{i(A)j(B)} = J$, a positive constant. The eigenvalues are readily calculated. The lowest energy belonging to each spin is given by $E(S)$, for $S \geq \mathcal{S}$, and the ground state belongs to $S = \mathcal{S}$.

$$E(S) = J\{S(S+1) - S_A(S_A+1) - S_B(S_B+1)\} \quad \text{for} \quad S \geq \mathcal{S}. \tag{20}$$

By the previous arguments, the ground-state eigenfunctions of this special Hamiltonian in a given M subspace satisfy Eq. (18) or (19) and are therefore not all orthogonal to the corresponding ground state of H. The special Hamiltonian has an $S = M$ ground state in each M subspace, provided $M \geq \mathcal{S}$. Therefore, so does H and this completes the proof for $g^2 = 0$.

When $g^2 > 0$, we have proved the theorem (4) for $H - g^2\mathbf{S}^2$ and it is therefore true *a fortiori* for H. However, the lowest ground state no longer necessarily belongs to $\mathcal{S}$, but belongs to $S \leq \mathcal{S}$.

MAGNETIC FIELD

A magnetic field in the z direction but of arbitrary and variable amplitude B_i modifies H_0 but not H_1, and therefore (18) or (19) are still valid for the ground state in an M subspace. The absolute ground state of the system is no longer necessarily in the $M \leq \mathcal{S}$ subspace nor is S a good quantum number in the presence of such a magnetic field.

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Magnetic Properties of Some Itinerant-Electron Systems at $T > 0$

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The Lieb-Mattis theorem on the absence of one-dimensional ferromagnetism is extended here from ground states to $T > 0$ by proving, *inter alia*, that $M(\beta,h)$, the magnetization of a quantum system in a field $h > 0$, is always *less* than the pure paramagnetic value $M_0(\beta,h) = \tanh(\beta h)$, with $\beta \equiv 1/kT$. Our proof rests on a new formulation in terms of path integrals that holds in any dimension; another of its applications is that the Nagaoka-Thouless theorem on the Hubbard model also extends to $T > 0$ in the sense that $M(\beta,h)$ *exceeds* $M_0(\beta,h)$.

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To many physicists the study of magnetism begins with a Heisenberg model, or something similar, in which localized spins interact with each other. Unfortunately, nature does not present us with such a starting point. Instead, at a reasonably (though not absolutely) fundamental level, we are presented with the Schrödinger equation for electrons whose interaction is, to a very good approximation, spin independent. It is left to the Pauli principle to induce a spin dependence, and for this it is essential that the electrons are *itinerant*, i.e., *not* localized *a priori*.

Given the subtlety of the phenomenon, it is crucial to elucidate the conditions which encourage or discourage the emergence of ferromagnetism. Some years ago Lieb and Mattis[1] showed that one *never* gets ferromagnetism in the ground states of itinerant electrons on a line. The results presented here include an extension of that earlier theorem (by a different method) to positive temperatures, and an opposite statement for systems in any dimension with a certain *parity constraint* (requiring *hard-core* repulsions)—for which we show that parallel spin alignments *are* favored at all temperatures. Examples of the second kind are one-dimensional systems of odd numbers of electrons on a ring (i.e., *periodic* boundary conditions), for which we extend the $T = 0$ result of Herring,[2] and a particular case of the Hubbard model whose ground state was shown to be ferromagnetic by Nagaoka[3] and Thouless.[4,5]

We deal with the following general (spin-independent) Hamiltonian for N identical, itinerant particles of mass m ($\hbar = 1$):

$$H = -(2m)^{-1}\sum_{i=1}^{N}\nabla_i^2 + V(x_1,x_2,\ldots,x_N), \qquad (1)$$

where V is some potential-energy function[6] which is symmetric in its N variables. Boundary conditions are stated below. We consider simultaneously (a) the continuum model (as just stated) and (b) the lattice model in which the x_i's have integer components and ∇^2 is the second difference operator.

If the particles are spin-$\frac{1}{2}$ fermions (e.g., electrons), the eigenstates of H can be classified according to the eigenvalues (j,s) of the total spin angular momentum operator J and of S—the z component ($j = N/2, N/2-1,\ldots,0$ or $\frac{1}{2}$, and $|s| \le j$). The eigenvalues of H depend on j but (for j specified) not on s. The ground-state energies are denoted by $E_0(j)$. Two simple benchmarks are the following: (i) Immobile, noninteracting, particles—with $m \to \infty$ and $V = 0$. In this limit $E_0(j)$ is *independent* of j. The system is a *pure paramagnet*, with spins responding to a magnetic field independently of each other. (Recall that $S = \sum\sigma_i^z/2$.) In a uniform field, $\mathbf{h} = (0,0,h)$, the partition function $Z(\beta,h) = \mathrm{Tr}\exp[-\beta(H - \sum\mathbf{h}\cdot\sigma_i)]$ satisfies

$$Z(\beta,h)/Z(\beta,h=0) \equiv \langle e^{2\beta hS}\rangle_{h=0} = [\cosh(\beta h)]^N$$

in this limit, and the magnetization is

$$M(\beta,h) = d[\ln Z(\beta,h)]/d(\beta h) = N\tanh(\beta h). \qquad (2)$$

(ii) Noninteracting itinerant system, with $V = 0$ and $0 < m < \infty$. The spectrum can be analyzed in terms of one-particle states, and one finds

$$E_0(j+1) > E_0(j) \qquad (3)$$

for all $j < N/2$. Thus, the "noninteracting" itinerant system shows a tendency towards *anti*ferromagnetism (resulting from the Pauli principle, which allows two electrons to occupy the same one-particle eigenstate of ∇^2 only if their spins are antialigned). At $T = 0$ and weak field the magnetization is 0 or 1.

The theorem of Lieb and Mattis[1] states that (3) always holds in 1D, even when $V \neq 0$. Although the theorem has some practical value for one-dimensional systems, its main conceptual value lies in the observation that theories of ferromagnetism based naively on Heisenberg's "exchange integral" can be misleading since two-body potentials with either ferromagnetic or antiferromagnetic exchange integrals can easily be con-

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structed in one dimension.[7]

Equation (3) states that increasing the spin costs ground-state energy. The first aim of this paper is to provide similarly precise information about the free energy when the inverse temperature β is finite. We denote the partition function with the trace restricted to subspaces with specified values of j, s, or both by $Z_{JS}(\beta, h;j,s)$, $Z_S(\beta,h;s)$, and $Z_J(\beta,h;j)$. When h is omitted, it is understood to take the value $h=0$. We also denote by $Y_{JS}^{(N)}(j,s)$, $Y_J^{(N)}(j)$, and $Y_S^{(N)}(s)$, the dimensions of these spaces for N noninteracting spins. The Y's [see (9) *et seq.*] serve as natural normalization constants for the Z's [because Eqs. (4) and (5) become equalities in the pure paramagnetic case].

Theorem 1.—Let N spin-$\frac{1}{2}$ fermions have the Hamiltonian (1) (with $m<\infty$) in a bounded region $[-L,L]^N$, with Dirichlet ($\psi=0$), Neumann ($\psi'=0$), or sticky [$\psi'/\psi(\pm L)=\lambda_\pm$] boundary conditions (either in the continuum or on a lattice). Then, for $\beta<\infty$,

$$Z_S(\beta;s+1)/Y_S^{(N)}(s+1) < Z_S(\beta;s)/Y_S^{(N)}(s)\,, \tag{4}$$

$$Z_J(\beta;j+1)/Y_J^{(N)}(j+1) < Z_J(\beta;j)/Y_J^{(N)}(j)\,, \tag{5}$$

for all j and $s\geq 0$. In a field $h>0$ the magnetization satisfies

$$0<M(\beta,h)<N\tanh(\beta h)\,. \tag{6}$$

Furthermore, there are strictly positive functions C_N, $C_{N-2}, C_{N-4}, \ldots, C_0$ or C_1 (which depend on β but not on s) such that, for $|s|\leq N/2$,

$$Z_S(\beta;s)=\sum_{k=0}^{N} C_k(\beta)Y_S^{(k)}(s)\,, \tag{7}$$

and

$$Z(\beta,h)=\sum_{k=0}^{N} C_k(\beta)[\cosh(\beta h)]^k\,, \tag{8}$$

where it is understood that $C_k\equiv 0$ if $N-k$ is odd, and $Y_S^{(k)}(s)\equiv 0$ if $k<2|s|$.

Remarks.—(1) Equations (7) and (8) are equivalent. They assert that, as far as the total spin is concerned, the thermal equilibrium state is effectively a (positive) superposition of states corresponding to systems of fewer (k) spins with no interaction.

(2) It is false that the susceptibility $\chi(h)\equiv\beta^{-1}\partial M(\beta,h)/\partial h$ does not exceed the pure paramagnetic value $N\cosh^{-2}(\beta h)$. By an elementary calculation using (8), the opposite is *always* the case for *very large* h (with the threshold possibly dependent on N).

(3) Equation (8) is derived below from (13); before turning to it let us note that (4) and (5), which are *not* derivable from each other, follow from (7) by elementary algebra. To do that, let us first recall that by the theory of angular momentum, for $|s|\leq j$,

$$\begin{aligned} Z_{JS}(\beta;j,s)&=Z_{JS}(\beta;j,j)=Z_S(\beta;j)-Z_S(\beta;j+1)\\ &=Z_J(\beta;j)/(2j+1)\,. \end{aligned} \tag{9}$$

Similar identities hold for $Y_{JS}^{(N)}(j,s)$, $Y_J^{(N)}(j)$, and $Y_S^{(N)}(s)$, with $Y_S^{(N)}(s)=N!/(N/2+s)!(N/2-s)!$.

To derive (4) from (7), one needs to establish the monotonicity in $|s|$ of $Y_S^{(k)}(s)/Y_S^{(N)}(s)$, for $N-k>0$ even. To do that, it is convenient to write this ratio as a telescopic product, whose factors are the monotone functions

$$Y_S^{(k)}(s)/Y_S^{(k+2)}(s)=[(k/2+1)^2-s^2]/(k+2)\,.$$

Equation (5) is derived by a similar tactic. Equation (6) is an elementary consequence of (8).

In Theorem 1 it is assumed that the interaction has no hard-core repulsion, or other singularities which are strong enough to induce nodal surfaces in the configuration space. The only role of this assumption is to allow (4)–(6) to be stated as *strict* inequalities. For our second result we let H include such repulsive interactions, which are the *sine qua non* for the *parity restriction* which is essential for Theorem 2. The term "dynamically allowed" refers there to those permutations that can be achieved by a motion of the particles that does not pass through a nodal surface induced by the positive divergence of the potential. For example, in 1D permutations are restricted if the interaction includes a hard-core repulsion which disallows particle encounters.

Theorem 2.—Suppose that in a system of N spin-$\frac{1}{2}$ fermions with Hamiltonian (1), in arbitrary dimension and in the continuum or on a lattice, the dynamically allowed permutations are all *even* and not restricted to the identity. (This parity requirement can be satisfied only if H includes a *hard-core repulsion.*) Then: (i) Among the ground states there is one with $j=N/2$. (ii) In a field $h>0$ the magnetization satisfies

$$M(\beta,h)>N\tanh(\beta h)\,. \tag{10}$$

(iii)

$$Z(\beta,h)=\sum_{\{n\}:\sum n_i=N} D_{\{n\}}(\beta)\prod_i \cosh(\beta h n_i) \tag{11}$$

for some $D_{\{n\}}(\beta)\geq 0$, with $\{n\}=\{n_1,n_2,\ldots\}$ varying over partitions of N. $D_{\{n\}}(\beta)>0$ if and only if there is an allowed permutation whose cycle lengths are $n_1,n_2,\ldots$.

Remarks.—(1) The content of (11) is that as far as the z-component S is concerned, at thermal equilibrium the system is in a superposition of states in which the particles form independent "cliques" of sizes n_i whose contribution to S is $\pm n_i/2$. In such a state the system shows enhanced response to magnetic fields. In particular, Eq. (10) [which should be contrasted with (6)] follows from (11) by writing $M(\beta,h)=E(\sum_j n_j \times\tanh(\beta h n_j))$, where $E(\cdot)$ is a normalized average over partitions with weights proportional to $D_{\{n_i\}} \times\prod_i\cosh(\beta h n_i)$, and applying the strict monotonicity of $\tanh(\cdot)$. By a similar argument, all the moments $\langle S^k\rangle$ exceed their paramagnetic values. (A similar clique structure can be inferred for the ferromagnetic Ising model from the Fortuin-Kasteleyn[8] representation.) As-

sertion (i) follows from the uniform bound $Z_S(\beta,N/2)/Z(\beta) \geq 2^{-N}$, implied by (11).

(2) Two examples to which Theorem 2 applies are the following: (a) The Hubbard model in the strong-coupling limit, with one hole on a bipartite lattice. In this case part (i) [in the stronger sense that $E_0(j)$ is strictly lowest at $j=N/2$] was established by Nagaoka and Thouless.[3-5] Our contribution is to extend their result to positive temperatures, in the sense of (10). (b) Systems of *odd* numbers N of spin-$\frac{1}{2}$ fermions in a ring, i.e., in $[0,L]^N$ with periodic boundary conditions, and a *hard-core repulsion.* The dynamically allowed permutations are powers of the cyclic shift $P \equiv (1,2,\ldots,N)$, whose parity equals $(-1)^{N-1}=1$. Part (i) was proved in that case by Herring.[2] Herring's and our method also yield[9] $E_0(N/2-1) > E_0(N/2)$.

(3) Theorem 2 has a very restrictive hypothesis which is not satisfied in cases of direct physical interest. Its value lies in two points: (i) the light it sheds on the mechanism of ferromagnetism; (ii) the construction used in the proof, which introduces ideas not ordinarily encountered in the study of electron correlations, e.g., the notion of cliques and the representation (13) which is always valid regardless of the hypothesis.

We turn now to the proof of (8) and (11), by first analyzing the Feynman-Kac path-integral representation[10] of $\mathrm{Tr}\, e^{-\beta H}$:

$$Z(\beta,h) = \int_{\Omega_\beta} \rho(d\omega) \exp\left[-\int_0^\beta V(x(t))dt\right](-1)^{\pi(\omega)} \times \exp\left[\beta h \sum_{i=1}^N \sigma_i\right]. \quad (12)$$

Here, $\omega = \{(x(t),\sigma(t)) | 0 \leq t \leq \beta\}$, which we refer to as a "path," represents a trajectory of the N particles, with $x=(x_1,\ldots,x_N)$, $\sigma=(\sigma_1,\ldots,\sigma_N)$. Ω_β is the collection of paths such that (i) the spins $\sigma_i(t) = \pm 1$ are constant in time, i.e., independent of t; (ii) the particle configuration at time β is a permutation, $\pi(\omega)$, of the configuration at time zero, with $(-1)^{\pi(\omega)}$ the parity of that permutation; and (iii) there are no encounters of particles of equal spin. $\rho(d\omega)$ is a (*positive-*) probability measure on Ω_β, determined by just the kinetic component of H, which we now describe in more detail for the two cases considered here.

In the discrete case, with x_i taking values on some lattice, the particle trajectories are piecewise constant functions of time, and hop to neighboring sites independently and at random times. The jumps form a Poisson process, with the probability ρ that a specified particle does not jump during the time interval $t \in [a,b]$ given by $\exp(-|a-b|m)$.

In the continuum case, $\rho(d\omega)$ is a product of Wiener measures constrained to satisfy the periodicity requirement (ii); i.e., $x(t)$ is a "Brownian bridge" with $x_i(\cdot)$ continuous in time. For the Dirichlet Laplacian the paths are killed at the boundary; for Neumann they are "reflected" (in a sense thoroughly discussed in textbooks).

The third condition is absent *a priori*, but it is a standard observation that its inclusion does not affect the value of the integral. (The proof of this version of the Pauli exclusion principle can be based on the symmetry transformation that exchanges the trajectories leading to the earliest equal-spin encounter.) A useful implication for us is that paths in Ω_β have no triple encounters; this follows from the other properties of Ω_β and the fact that the spins take only two values.

The measure in (12) possesses a hidden symmetry which we shall uncover. We are going first to define for each path ω a collection $\Gamma(\omega)$ of loops γ. Each loop will have a winding number $w(\gamma)$. There will be a symmetry group $\mathcal{G}$ having 2^N elements each of which maps Ω_β in a one-to-one way onto Ω_β preserving $\Gamma(\omega)$, $\rho(d\omega)$, $\int V(x(t))dt$, and $(-1)^{\pi(\omega)}$. However, $\mathcal{G}$ does not preserve $\pi(\omega)$ and the spin values $s=\sum\sigma_i$. The values attained by s within the ensemble of paths related by the action of $\mathcal{G}$ are of the form $\sum_{\gamma\in\Gamma(\omega)} \pm w(\gamma)/2$, with all the configurations of $\pm$ signs occurring with equal weights. Symmetrization of the integrand in (12) then yields the following useful representation:

$$Z(\beta,h) = \int_{\Omega_\beta} \rho(d\omega) \exp\left[-\int_0^\beta dt\, V(x(t))\right](-1)^{\pi(\omega)} \times \prod_{\gamma\in\Gamma(\omega)} \cosh[\beta h w(\gamma)]. \quad (13)$$

The loops are associated with the space-time picture of the collection of particle trajectories of the path ω (see Fig. 1). They are drawn by starting from the $t=0$ location of any of the particles, and tracing the particle's location forward in space-time until its first encounter with another particle; at which point the tracing line switches to the world line of the other particle in the reversed orientation in time. Such an orientation switch is repeated whenever a particle encounter is reached. When the trace line reaches the time $t=0$ or β, it reemerges at the

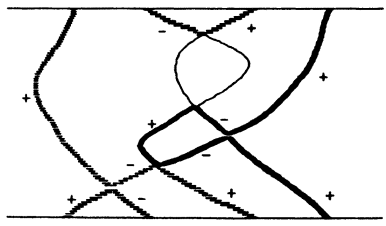

FIG. 1. This collection of particle world lines has two loops with winding numbers $\{1,1\}$. The statistical distribution of s under the symmetry group is that of two noninteracting spin-$\frac{1}{2}$ particles. In dimensions $d > 1$, and for 1D periodic boundary conditions, permutations can occur without there being particle encounters, and then the winding numbers can be larger.

same location with time treated as periodic. This is continued until a loop is closed. For each $\omega \in \Omega_\beta$ the loops will all have only finite numbers of orientation reversals, since that number can diverge only if there is a triple encounter. We denote the collection of the distinct loops (γ) by $\Gamma(\omega)$, and define $w(\gamma)$ to be the absolute value of the loop's winding number, i.e., $w(\gamma) = |\int_\gamma dt/\beta|$.

A path $\omega \in \Omega_\beta$ is completely characterized by three things: the initial configuration $x(0)$, the union of the world lines, and the spin assignments along the world lines. It is evident that consistency with the constraints (i)–(iii) is achieved if and only if the spin assignment alternates along each loop, as shown in Fig. 1. By this condition, reading along the $t=0$ line, the admissible values of $2s$ are of the form $\sum_i \sigma_i = \sum_{\gamma \in \Gamma(\omega)} \pm w(\gamma)$.

We now define the group $\mathcal{G}$ to have N commuting generators g_i. In the space-time picture the map g_i flips the spin values $(+\frac{1}{2} \leftrightarrow -\frac{1}{2})$ along the loop γ containing the $t=0$ position of the ith particle. The spin flip is accompanied by the unique rearrangement of particle trajectories needed to maintain the constraints (i)–(iii). The paths ω and $g_i\omega$ differ in the $\pm$ sign attached to $w(\gamma)$.

To show that g_i preserves the parity of $\pi(\omega)$, we note that $\pi(g_i\omega)$ is obtained from $\pi(\omega)$ by a product of transpositions associated with the orientation reversals in the loop γ; their number is always even. The invariance of $\rho(d\omega)$ is evident in the lattice case with discrete time steps. The invariance in the continuum case can be deduced by verifying that g_i are continuous maps in the uniform topology of Ω_β and invoking Donsker's theorem[11] on the weak convergence of the random-walk measures to the Wiener measure.

Equation (13)→(8): Evidently, on a line $\pi(\omega)$ can only be the identity, and $w(\gamma)$ can only take the values 0 and 1. Then (13) directly implies (8) with $C_k(\beta)$ given by the integral in (13) restricted to ω's for which the number of loops with $w(\gamma)=1$ is exactly k. The strict positivity is assured by the nonvanishing contributions from paths ω with collisions occurring only within the first $(N-k)/2$ pairs of adjacent particles. Q.E.D.

Equation (13)→(11): The hard-core repulsion precludes encounters, so the loops are dynamically simple but have nontrivial winding numbers, satisfying $\sum w(\gamma) = N$. Q.E.D.

Finally, we remark that Theorem 1 admits a *parastatistical* extension—as did the ground-state theorem of Ref. 1.

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$$\sup_x \int_{|y| \le a} d^{Nd}y \|y\|^{-(Nd-2)} |V(y-x)| \to 0$$

as $a \to 0$. If V consists of k-body interaction, that condition translates to a lower-dimensional condition of similar form, with the weight becoming $\ln\|y\|$ for $kd=2$, and 1 for $kd=1$.

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Part V

Laser Models

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Phase Transitions in Reservoir-Driven Open Systems with Applications to Lasers and Superconductors

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Abstract. We present a class of mean field model Hamiltonians consisting of a small, but macroscopic system S of N components interacting with a large reservoir R. The Dicke model of a laser is a particular example of S. Both R and S are fully quantum mechanical. The exact equations of motion are studied, and it is shown that it is possible to eliminate the reservoir variables and, in the limit $N \to \infty$, to derive closed equations for the extensive variables of S. These equations are classical, and the effect of the reservoir is to provide damping and driving (or pumping) terms. As the parameters of the system are varied, S can undergo phase transitions in the sense that its equilibrium orbits bifurcate. To the next order, $N^{1/2}$, the reservoir drives the fluctuation observables of S linearly with Markovian, Gaussian random forces. Within the context of our class of models our results are rigorous and are obtained without any approximation.

1. Introduction

The Dicke–Haken–Lax model of the finite mode laser [D1], [H1], [L2] is interesting both for equilibrium and non-equilibrium statistical mechanics. Not only is it supposed to have some relevance to the real world, but from the theoretical point of view it provides an exactly soluble model with non-trivial consequences. The structure of the model without losses is such that to leading order in N (the number of atoms) the equations of motion for the expectation values of extensive observables are classical, while to the next order, $N^{1/2}$, quantum effects become manifest. It was because of this clean separation of quantum and classical effects that we were able to deduce exactly the equilibrium thermodynamic properties of the 1-mode laser in the rotating wave approximation [H4] and were later able to generalize those results by permitting several photon modes, eliminating the rotating wave approximation and even dispensing with the necessity of spatial homogeneity of the atoms [H5], [H7], [W1].

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In this paper we take the next step which is to elucidate the properties of a laser coupled to a reservoir. On the basis of our previous work we expect that the primary effect of the reservoir will be to provide a simple damping for the laser and at the same time to drive the extensive quantities of the laser to new stationary, non-equilibrium values, when the coupling or pumping constant exceeds a critical value. Again, to leading order in N, the new equations for the extensive observables should be classical and the residual quantum effects of the reservoir should be manifest only to order $N^{1/2}$ as fluctuation forces which should drive the laser fluctuation observables linearly about their mean values. If one assumes this to be true, then one has precisely the theory of the laser developed by others, except near the critical point, where the limit $N \to \infty$ is not interchangeable with the limit time $\to \infty$. The problem is to validate the above assumptions, and it is to this to which this paper is devoted. If one looks at the equations of motion for the laser and the reservoir operators, the above-mentioned N-dependence is at once clearly seen to be consistent with those equations but, because the reservoir is huge compared to the laser, it is quite another matter to *prove* that the effect of the reservoir is really as tame as it would appear to be. Since different reservoirs can produce different stationary states for the laser, the reservoir is of paramount importance to the laser.

One might turn the question around by saying that the problem is to find a large system which, when coupled to the laser, behaves the way a reservoir is intuitively expected to behave according to the phenomenological equations of semi-classical theory. There are some analogies to the construction of a sensible macroscopic measuring apparatus in the theory of quantum mechanical measurement [H3]. In this paper we actually construct a proper reservoir. It is built of fermions and some objects not readily obtainable from the laboratory shelf, but it shows that the phenomenological equations are consistent with at least one microscopic model. In the future we hope to be able to provide more realistic reservoirs.

A typical Hamiltonian for the laser system S that one might wish to consider is

$$H^S_{(N)} = \nu a^* a + \epsilon S^3_{(N)} + \lambda N^{-1/2}(S^+_{(N)} a + S^-_{(N)} a^*) + \mu N^{-1/2}(S^+_{(N)} a^* + S^-_{(N)} a). \tag{1.1}$$

If $\mu = 0$, (1.1) is the 1-mode Dicke model in the rotating wave approximation. a^* are the creation and annihilation operators for a single photon mode, and $S^i_{(N)} = \sum_{n=1}^N S^i_n$, $i = 1, 2, 3$, are the total 'spin' operators for N 2-level atoms ($\underline{S}_n$ is a spin $\frac{1}{2}$ operator). The physical interpretations of $S^3_{(N)}$ is that of the total atomic inversion operator, while $S^*_{(N)} = S^1_{(N)} < iS^2_{(N)}$ are proportional to the total polarization operators. The inclusion of more than one photon mode and of multi-level atoms without spatially dependent coupling constants to the radiation field does not vitiate our methods, it only makes the resulting equations and their properties more complicated. The closed system properties of such a Hamiltonian (1.1) have been discussed by us previously [H4], [H5] and by many others [S2], [S3], [T1], [W1].

The reservoirs we shall consider consist of separate systems for each atom and each photon mode. A desirable photon reservoir would itself consist of bosons [S5], i.e.

$$H^R = \int dw E(w)\, A^*_w A_w + \int dw (k(w)\, A^*_w a + \text{h.c.}), \tag{1.2}$$

where A_w, $w \in \mathbf{R}$, is a boson field with $[A_w, A^*_{w'}] = \delta(w - w')$, and the initial state of the reservoir is, for instance, the vacuum. The reservoir for a single atom could be imagined to consist of a large number of 2-level atoms [S1] in a state of inverted population which, by a suitable coupling, has the effect of pumping the laser atoms. It is well known

that the excitations of such an ensemble of atoms are boson-like, so we may as well eliminate a needless difficulty by assuming *ab initio* that the atom reservoir does indeed consist of bosons, i.e. for the nth atom

$$H_n^A = \int dw F(w)[B_{nw}^* B_{nw} + C_{nw}^* C_{nw}] + \int dw[g_B(w) B_{nw}^* S_n^- + g_C(w) C_{nw}^* S_n^+ + \text{h.c.}], \tag{1.3}$$

where $B_{nw}^\#$ and $C_{nw}^\#$ are two boson fields. The B-field pumps the atom down and the C-field pumps it up. Actually, the reservoirs we shall consider in Section 5 are similar to (1.3), but are mathematically more tractable.

The full Hamiltonian [H1], [L2] is

$$H_{(N)} = H_{(N)}^S + H_{(N)}^R, \quad H_{(N)}^R = H^P + \sum_{n=1}^{N} H_n^A. \tag{1.4}$$

For any operator, A, $A(t) = \exp(iHt) A \exp(-iHt)$. (We drop the subscript N, whenever it is not absolutely necessary.) The equations of motion for the A-, B- and C-field operators are easy to derive and are linear, and can be solved in terms of the $(t=0)$-operators and the photon and atom operators. Inserting these solutions into the equations of motion for the latter operators, one finds (with $\dot{A} = dA/dt$)

$$\dot{a}(t) = -i\nu a(t) - i\lambda N^{-1/2} S_{(N)}^-(t) - i\mu N^{-1/2} S_{(N)}^+(t) - \int_0^t ds \kappa(t-s) a(s) + f(t), \tag{1.5}$$

$$\dot{S}_n^+(t) = i\epsilon S_n^+(t) - 2i\lambda N^{-1/2} S_n^3(t) a^*(t) - 2i\mu N^{-1/2} S_n^3(t) a(t) + 2\int_0^t ds \gamma_B(t-s) S_n^+(s) S_n^3(t) - 2\int_0^t ds \gamma_C(t-s) S_n^3(t) S_n^+(s) + G_n^+(t), \tag{1.6}$$

$$\dot{S}_n^3(t) = (-i\lambda N^{-1/2} S_n^+(t) a(t) - i\mu N^{-1/2} S_n^+(t) a^*(t) + \text{h.c.}) + \int_0^t ds[\gamma_C(t-s) S_n^-(t) S_n^+(s) - \gamma_B(t-s) S_n^+(s) S_n^-(t) + \text{h.c.}] + G_n^3(t) \tag{1.7}$$

and

$$f(t) = -i \int dw k^*(w) A_w \exp(-iE(w) t), \tag{1.8}$$

$$\begin{aligned} G_n^+(t) &= -2i \int dw g_B(w) B_{nw}^* S_n^3(t) \exp(iF(w) t) \\ &\quad -2i \int dw g_C^*(w) S_n^3(t) C_{nw} \exp(-iF(w) t), \\ G_n^3(t) &= i \int dw g_B(w) B_{nw}^* S_n^-(t) \exp(iF(w) t) \\ &\quad -i \int dw g_C(w) C_{nw}^* S_n^+(t) \exp(iF(w) t) + \text{h.c.} \end{aligned} \tag{1.9}$$

In the above

$$\kappa(t) = \int dw |k(w)|^2 \exp(-iE(w) t), \tag{1.10}$$

$$\gamma_B(t) = \int dw |g_B(w)|^2 \exp(iF(w) t), \tag{1.11}$$

$$\gamma_C(t) = \int dw |g_C(w)|^2 \exp(-iF(w) t). \tag{1.12}$$

In (1.5) and (1.6), the operators $f(t)$ and $G_n(t)$ have the property that their (partial) expectation value in the reservoir vacuum is zero. For that reason we call them *fluctuation forces*. f is explicitly given and is of $O(1)$, and the main problem is to show that $g^i_{(N)}(t) = N^{-1/2} \sum G^i_n(t)$ is also $O(1)$, where the precise meaning of $O(1)$ for these unbounded operators will be explained later. If f is truly $O(1)$ and if $S^-_{(N)}$ is $O(N)$ and a is $O(N^{1/2})$, then there is no objection to dropping f in (1.5). However, in (1.6) G^+_n is $O(1)$, and it has a profound influence on S^+_n, which is also $O(1)$. In fact, it is an essential ingredient in preserving the norms and the commutation relations of the $S^i_n(t)$. The hope would be that one could find an equation for the total $S^i_{(N)}(t)$, in which the total fluctuation force $N^{1/2} g^i_{(N)}$, which is $O(N^{1/2})$, can be dropped. This suggests summing (1.6) over n and dividing by N. Unfortunately this does not yield a closed equation for $S^i_{(N)}(t)$; it would do so, if γ_B and γ_C were Dirac delta functions. If γ_B and γ_C are *not* delta functions (which case we shall term the *regular* reservoir) a more subtle procedure is required to obtain an equation for $S^i_{(N)}(t)$. In a subsequent paper we shall deal with that question. For now, we suppose that γ_B, γ_C and κ are indeed proportional to delta functions. This requires choosing

$$E(w) = F(w) = w, \quad g_B(w) = g_B, \quad g_C(w) = g_C \quad \text{and} \quad k(w) = k.$$

Such a reservoir is called *singular*, because its energy has neither an upper nor a lower bound and the Hamiltonian is in general only defined as a bilinear form and not as an operator. In Section 3 we shall give a meaning to the time evolution of systems coupled to singular reservoirs.

With this assumption we can now sum (1.6) over n and, recalling that $S^3_n(t) S^+_n(t) = S^+_n(t)/2$, and introducing the intensive observables

$$\alpha_{(N)}(t) = N^{-1/2} a_{(N)}(t),$$
$$\sigma^i_{(N)}(t) = N^{-1} S^i_{(N)}(t), \tag{1.13}$$

one finds

$$\dot{\alpha}_{(N)}(t) = -(i\nu + \kappa)\, \alpha_{(N)}(t) - i\lambda \sigma^-_{(N)}(t) - i\mu \sigma^+_{(N)}(t) + \varphi_{(N)}(t), \tag{1.14}$$

$$\dot{\sigma}^+_{(N)}(t) = (i\epsilon - \gamma)\, \sigma^+_{(N)}(t) - 2i\lambda \sigma^3_{(N)}(t)\, \alpha^*_{(N)}(t) - 2i\mu \sigma^3_{(N)}(t)\, \alpha_{(N)}(t) + \chi^+_{(N)}(t), \tag{1.15}$$

$$\dot{\sigma}^3_{(N)}(t) = -2\gamma(\sigma^3_{(N)}(t) - \eta) + \chi^3_{(N)}(t) + [i\lambda \sigma^-_{(N)}(t)\, \alpha^+_{(N)}(t) + i\mu \sigma^-_{(N)}(t)\, \alpha_{(N)}(t) + \text{h.c.}], \tag{1.16}$$

where

$$\eta = [|g_C|^2 - |g_B|^2]/2[|g_C|^2 + |g_B|^2] \tag{1.17}$$

is the pumping rate (which can vary between $-\frac{1}{2}$ and $\frac{1}{2}$), and

$$\gamma = \pi[|g_C|^2 + |g_B|^2], \tag{1.18}$$

$$\kappa = \pi |k|^2 \tag{1.19}$$

are damping constants.

Equations (1.14)–(1.16) are the desired equations of motion for the intensive observables. As the commutators of $\sigma^i_{(N)}$ and $\alpha^\#_{(N)}$ are $O(N^{-1})$, and as the fluctuation forces $\varphi_{(N)}, \chi^i_{(N)}$ are hopefully $O(N^{-1/2})$, we expect that (1.14)–(1.16) go over into classical equations in suitable states (which we shall call 'classical' in Section 2).

The nature of the solutions of this non-linear equation (1.14)–(1.16) (in the classical limit) can be expected to depend sensitively on the parameters (damping constants and

pumping rate), and we shall give some physical examples in the last section. In particular, the laser threshold will be an example of a phase transition in a stationary, but non-equilibrium state. This interpretation of the laser threshold has been given before but without rigorous justification [D2], [G2], [S4].

We have written the above equations (1.1)–(1.19) to outline the steps one would like to follow from a microscopic Hamiltonian to a classical differential equation. It is plain that our justification, such as it was, for the various steps was at best circular and imprecise. It is to give a rigorous proof of the above expansion in powers of $N^{-1/2}$ that the rest of this paper is devoted. In so doing we shall give a non-trivial example of a microscopic quantum mechanical theory of macroscopic irreversibility and self-oscillatory behaviour, in a sense a model of a quantum mechanical steam engine. To be perfectly precise, however, the model we shall treat in the sequel is not exactly the same as (1.1)–(1.3), although it is hardly less physical and the classical equations are essentially the same as (1.14)–(1.16). The reason for the alteration is a technical one having to do with the unbounded nature of boson fields. In a later paper [H6] we shall return to the model (1.1)–(1.3), but here we study fermion reservoirs and introduce an arbitrarily large photon number cutoff proportional to N.

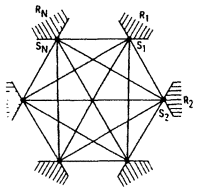

Figure 1
Structure of a system $S = \{S_1, \ldots S_N\}$ with mean field interaction and independent reservoirs $R = \{R_1, \ldots R_N\}$.

Sections 2, 3 and 4 give a systematic account of dissipative fermion systems with non-linear mean field type interaction of the symbolic structure depicted in Figure 1. The setting is somewhat abstract, but we believe that this has the advantage of clarifying the fundamental mathematical ideas behind the proofs. The main theorems have clear intuitive meaning, and they are not pushed to utmost generality. Chapter 5 gives the application of the general theory to various physical systems, namely to the laser and to a system consisting of two strongly coupled superconductors, the reservoir driven, mean-field Josephson effect.

2. Classical Limits in Mean Field Models

In this section we consider a large number, N, of identical subsystems coupled together by a mean field-like Hamiltonian. Clearly, the relevant operators do not have limits as $N \to \infty$ in a strong sense, but their expectation values do have limits in certain states (which might typically be the ground state or Gibbs states [H4], but not necessarily so). We shall characterize states in which a polynomial algebra of macroscopic observables have reasonable physical homogeneity properties, as classical with respect to these observables, and the precise definition of this concept is given below. The problem is to show that if the expectation values are classical at time zero, that

they continue to be classical for all times, and that expectation values (Wightman or Green functions) obey simple classical equations. A similar problem arises, if one starts with initial conditions where the fluctuations of relevant observables around the classical values are normal. Do they continue to be normal, and are the resulting equations of motion linear as one expects from the theory of ordinary differential equations?

In the following, each $\mathscr{A}_n$ is a collection of operators which act on one of the identical subsystems, and it can be imagined to be all linear operators on a finite dimensional complex vector space. This space might, for example, be the internal states of several multi-level atoms with a fixed number of electrons.

Let $\mathscr{A}_n$, $n \in \mathbf{Z}$ (all integers) be a countable family of C^*-algebras, where each $\mathscr{A}_n \simeq \mathscr{B}(\mathbf{C}^K)$ is isomorphic to the set of all linear operators on a fixed $\mathbf{C}^K$. For $m \neq n$, $[\mathscr{A}_m, \mathscr{A}_n] = 0$. Let $\mathscr{A}$ be the quasilocal C^*-algebra generated by $\bigcup \mathscr{A}_n$[R2]. (There are obvious generalizations to fancier quasilocal structures.) Let τ be a representation of $\mathbf{Z}$ as translation automorphisms of $\mathscr{A}$. Let $A \in \mathscr{A}_0$ and

$$\alpha_{(N)} = N^{-1} \sum_{n=1}^{N} \tau_n A. \tag{2.1}$$

$\alpha_{(N)}$ is called an intensive observable of first degree. (A more general class of averages has been studied by [K1], [R3].) Let $A^1, \ldots A^L$ be a basis of $\mathscr{A}_0$ ($L = K^2$) and $\alpha^1_{(N)}, \ldots \alpha^L_{(N)}$ the corresponding intensive observables. A polynomial $\beta_{(N)} = \beta(\alpha^1_{(N)}, \ldots \alpha^L_{(N)})$ is called an intensive polynomial. If

$$\gamma_{(N)} = \gamma(\alpha^1_{(N)}, \ldots \alpha^L_{(N)}) = n - \lim_{m\to\infty} \beta^m(\alpha^1_{(N)}, \ldots \alpha^L_{(N)}) \tag{2.2}$$

uniformly in N with fixed intensive polynomials $\beta^m_{(N)}$, then $\gamma_{(N)}$ is called an intensive observable.

An extensive observable, $A_{(N)}$, is N times an intensive observable, $A_{(N)} = N\alpha_{(N)}$. For every $\alpha \in \mathbf{C}$

$$a_{(N)} = \sqrt{N}(\alpha_{(N)} - \alpha) \tag{2.3}$$

is called the fluctuation observable of $\alpha_{(N)}$ around α.

For intensive polynomials $\alpha_{(N)}$ and $\beta_{(N)}$ (and more generally for a large class of intensive observables of the type (2.2)), $[\alpha_{(N)}, \beta_{(N)}] = O(N^{-1})$ for $N \to \infty$. Hence these operators are candidates for classical observables, while the fluctuation operators could become boson operators with c-number commutators in the limit $N \to \infty$. The limit $N \to \infty$ cannot be discussed in $\mathscr{A}$, but it is meaningful in certain states of $\mathscr{A}$ which we now describe.

Let $\mathscr{L}$ be a self-adjoint Lie subalgebra of $\mathscr{A}_0$ with real basis $A^1, \ldots A^l$. All future statements will be made relative to $\mathscr{L}$.

A state ω of $\mathscr{A}$ is called classical (with respect to $\mathscr{L}$) if, for *all* intensive polynomials $\beta_{(N)} = \beta(\alpha^1_{(N)}, \ldots \alpha^l_{(N)})$,

$$\lim_{N\to\infty} \omega(\beta_{(N)}) = \langle\beta\rangle_\omega \tag{2.4}$$

exists. Then there exists [R3] a probability measure μ_ω on the 'phase space' $\mathbf{R}^l$ with support in $|\alpha^k| \leqslant \|A^k\|$, $1 \leqslant k \leqslant l$, such that for all monomials

$$\lim_{N\to\infty} \omega((\alpha^1_{(N)})^{m(1)} \ldots (\alpha^l_{(N)})^{m(l)}) = \int \mu_\omega(d\alpha)(\alpha^1)^{m(1)} \ldots (\alpha^l)^{m(l)}. \tag{2.5}$$

A state ω of $\mathscr{A}$ is called a pure classical state (with respect to $\mathscr{L}$), if μ_ω is concentrated on one point $\underline{\alpha} = (\alpha^1, \ldots \alpha^l) \in \mathbf{R}^l$; alternatively, if for all monomials

$$\lim_{N\to\infty} \omega((\alpha^1_{(N)})^{m(1)} \ldots (\alpha^l_{(N)})^{m(l)}) = \prod_{\lambda=1}^{l} (\alpha^\lambda)^{m(\lambda)}. \tag{2.6}$$

It is known [K1], [R3] that every translation invariant state ω on $\mathscr{A}$ is classical and ω is pure if it is an extremal point of all translation invariant states on $\mathscr{A}$.

A state ω on $\mathscr{A}$ has normal fluctuations with respect to $\underline{\alpha}_{(N)} = (\alpha^1_{(N)}, \ldots \alpha^l_{(N)})$ around $\underline{\alpha} \in \mathbf{R}^l$, if, for all monomials in $a^k_{(N)} = \sqrt{N}(\alpha^k_{(N)} - \alpha^k)$, $1 \leqslant k \leqslant l$, $s = 1, 2, \ldots$

$$\lim_{N\to\infty} \omega(a^{k(1)}_{(N)} \ldots a^{k(s)}_{(N)}) = \langle a^{k(1)} \ldots a^{k(s)} \rangle_\omega \tag{2.7}$$

exists. By the GNS construction there exists a Hilbert space $\mathscr{H}_\omega$ with a vector $\Omega_\omega \in \mathscr{H}_\omega$ which is cyclic with respect to the algebra of all polynomials in (possibly unbounded) linear operators $a^1_\omega, \ldots a^l_\omega$ on $\mathscr{H}_\omega$, such that

$$\langle a^{k(1)} \ldots a^{k(s)} \rangle_\omega = (\Omega_\omega, a^{k(1)}_\omega \ldots a^{k(s)}_\omega \Omega_\omega). \tag{2.8}$$

It is easy to see that a classical state with normal fluctuations around $\underline{\alpha}$ is pure with μ_ω concentrated on $\underline{\alpha}$ and that for all $1 \leqslant i, j \leqslant l$

$$[A^i, A^j] = \sum_{k=1}^{l} C^{ij}_k A^k \Rightarrow [a^i_\omega, a^j_\omega] = \sum_{k=1}^{l} C^{ij}_k \alpha^k. \tag{2.9}$$

Of course, not every pure classical state has normal fluctuations. Necessary and sufficient conditions for purity and normality can be expressed in terms of the truncated ω-expectation values. Those are defined recursively for $X^1, \ldots X^s \in \mathscr{A}$ by

$$\omega^T(X^1 \ldots X^s) = \omega(X^1 \ldots X^s) - \sum{}' \omega^T(X^{i(1)} \ldots X^{i(r)}) \ldots \omega^T(X^{j(1)} \ldots X^{j(t)}) \tag{2.10}$$

where $\sum'$ extends over all partitions of $\{X^1, \ldots X^s\}$ into more than one set and $\omega^T(x^i) = \omega(X^i)$. The relevant operators are the $A^k_n \equiv \tau_n A^k$ for $1 \leqslant k \leqslant l$ and $n = 1, 2, \ldots$. ω is pure, if and only if

$$\lim_{N\to\infty} N^{-1} \sum_{n=1}^{N} \omega(A^k_n) = \alpha^k, \quad 1 \leqslant k \leqslant l, \tag{2.11}$$

exists and for all $s \geqslant 2$

$$\lim_{N\to\infty} N^{-s} \sum_{n(1),\ldots n(s)=1}^{N} \omega^T(A^{k(1)}_{n(1)} \ldots A^{k(s)}_{n(s)}) = 0. \tag{2.12}$$

ω has normal fluctuations around $\underline{\alpha}$, if and only if

$$\lim_{N\to\infty} N^{-1/2} \sum_{n=1}^{N} \{\omega(A^k_n) - \alpha^k\} \tag{2.13}$$

exists and

$$\lim_{N\to\infty} N^{-s/2} \sum_{n(1),\ldots n(s)=1}^{N} \omega^T(A^{k(1)}_{n(1)} \ldots A^{k(s)}_{n(s)}) \tag{2.14}$$

exists ($s \geqslant 2$).

One sees that a translation invariant direct product state ω with $\omega^T(A^{k(1)}_{n(1)}, \ldots A^{k(s)}_{n(s)}) \equiv 0$ for $s \geqslant 2$, has normal fluctuations.

In the following theorem the assumption of $\mathscr{L}$ being a finite dimensional Lie algebra is important for the first time:

Theorem 2.1: Let the Hamiltonian $H_{(N)} = H^*_{(N)} = N\beta(\alpha^1_{(N)}, \ldots \alpha^l_{(N)})$ be an extensive polynomial (associated with $\mathscr{L}$). Define

$$\alpha^k_{(N)}(t) = \exp iH_{(N)}t)\, \alpha^k_{(N)} \exp(-iH_{(N)}t). \tag{2.15}$$

Then for all $1 \leqslant k \leqslant l$ and all $t \in \mathbf{R}$ the $\alpha^k_{(N)}(t)$ are intensive observables and they are uniformly approximated by

$$\alpha^k_{(N)}(t) = n - \lim_{n(0), \ldots n(r) \to \infty} \alpha^k_{(N)n(0)\ldots n(r)}(t). \tag{2.16}$$

The polynomials $\alpha^k_{(N)n(0)\ldots n(r)}$ in $\alpha^1_{(N)}, \ldots \alpha^l_{(N)}$ are recursively defined by (2.22) as iterative solutions of the integral equation

$$\alpha^k_{(N)}(t) = \alpha^k_{(N)}(s) + i\int_s^t dr[H_{(N)}(r), \alpha^k_{(N)}(r)]. \tag{2.17}$$

These solutions are entire analytic in t and uniformly bounded in N in a neighbourhood of the real t-axis.

Proof: For finite N, $H_{(N)} \in \mathscr{A}$, and $\alpha^k_{(N)}(t) \in \mathscr{A}$ is norm-continuous in t and satisfies $\|\alpha^k_{(N)}(t)\| = \|A^k\|$ for all t and all $1 \leqslant k \leqslant l$. Let $0 \leqslant r < s$ and let $X_{(r,s)}$ be the Banach space of all norm-continuous curves

$$x = \{\underline{x}(t) = (x^1(t), \ldots x^l(t)) \in \mathscr{A}^l,\ r \leqslant t \leqslant s\},$$
$$\|x\| = \sup_{r \leqslant t \leqslant s} \max_{1 \leqslant k \leqslant l} \|x^k(t)\|. \tag{2.18}$$

Let $\alpha = \max\|A^k\|$ and $X^{2\alpha}_{(r,s)} = \{x \in X_{(r,s)},\ \|x\| \leqslant 2\alpha\}$. For $\underline{z} \in \mathscr{A}^l$ and $x \in X_{(r,s)}$, we define $y = T_{(r,s)}(\underline{z}, x) \in X_{(r,s)}$ by

$$y^k(t) = z^k + \int_r^t du\beta^k(x^1(u), \ldots x^l(u)), \tag{2.19}$$

where

$$\beta^k(\alpha^1_{(N)}(u) \ldots \alpha^l_{(N)}(u)) \equiv i[H_{(N)}(u), \alpha^k_{(N)}(u)]$$

is a polynomial which can be computed using the Lie structure (2.9) of $\mathscr{L}$. It is easy to see that there exists some $d > 0$ such that, whenever $|r - s| \leqslant d$ and $\|\underline{z}\| = \max\|z^k\| \leqslant 3\alpha/2$, $T_{(r,s)}(\underline{z}, \cdot)$ is a contraction on $X^{2\alpha}_{(r,s)}$ with a Lipschitz constant $\frac{1}{2}$. Thus, for $0 \leqslant t \leqslant d$, we can use the contraction fixed-point theorem to approximate the solutions to (2.17), uniformly in N, by a sequence of intensive polynomials $\alpha^k_{(N)n}(t) = T^n_0(\underline{\alpha}_{(N)})^k(t)$, which are recursively defined (as elements of $X^{2\alpha}_{(r,s)}$) by

$$T^n_0(\underline{\alpha}_{(N)}) = T_{(0,d)}(\underline{\alpha}_{(N)}, T^{n-1}_0(\underline{\alpha}_{(N)})),$$
$$T^0_0(\underline{\alpha}_{(N)}) = \underline{\alpha}_{(N)}. \tag{2.20}$$

Since for all $m = 1, 2, \ldots$, $\|\underline{\alpha}_{(N)}(md)\| \leqslant \alpha$, one can use $\underline{\alpha}_{(N)}(md)$ to compute $\underline{\alpha}_{(N)}(t)$ for $md \leqslant t \leqslant (m+1)d$, by applying the fixed-point theorem. Let $T^n_m(\underline{z})$ be defined as in

(2.20), with $(0, d)$ replaced by $(md, (m+1)d)$ and $\underline{\alpha}_{(N)}$ by $\underline{z}$. We claim that for every $m = 0, 1, 2, \ldots$ and every $\epsilon > 0$ there exists some $K(m, \epsilon) < \infty$ such that for all $n(0), \ldots n(m) \geqslant K(m, \epsilon)$ and for all $md \leqslant t \leqslant (m+1)d$ and all N

$$\|\alpha^k_{(N)n(0)\ldots n(m)}(t) - \alpha^k_{(N)}(t)\| < \epsilon. \tag{2.21}$$

The $\alpha_{(N)n(0)\ldots n(m)}$ are recursively defined as elements in $X_{(md,(m+1)d)}$ by

$$\alpha_{(N)n(0)\ldots n(m)} = T_m^{n(m)}(\underline{\alpha}_{(N)n(0)\ldots n(m-1)}(md)), \tag{2.22}$$

where the recursion starts at (2.20). Since T_m is a contraction, one has for all n and for all $\underline{x}, \underline{y}$ with $\|\underline{x}\|, \|\underline{y}\| \leqslant 3\alpha/2$:

$$\|T_m^n(x) - T_m^n(y)\| \leqslant \|x - y\| + \tfrac{1}{2}\|T_m^{n-1}(x) - T_m^{n-1}(y)\| \leqslant 2\|x - y\|. \tag{2.23}$$

Given $m = 0, 1, \ldots$ and $\epsilon > 0$, there exists some $K(m, \epsilon) < \infty$, such that for all $n(0), \ldots n(m) \geqslant K(m, \epsilon)$ and for all $\mu = 0, 1, \ldots m$

$$\|\underline{\alpha}_{(N)} - T_\mu^{n(\mu)}(\underline{\alpha}_{(N)}(\mu d)\| < \epsilon 2^{m-\mu}(m+1)^{-1} \tag{2.24}$$

as elements of $X^{2\alpha}_{(\mu d,(\mu+1)d)}$. Hence, by (2.23),

$$\begin{aligned}\|\alpha_{(N)} - \alpha_{(N)n(0)\ldots n(m)}\| &\leqslant \|\alpha_{(N)} - T_m^{n(m)}(\underline{\alpha}_{(N)}(md))\| \\ &+ \|T_m^{n(m)}(\underline{\alpha}_{(N)}(md)) - T_m^{n(m)}(\underline{\alpha}_{(N)n(0)\ldots n(m-1)}(md))\| < \epsilon(m+1)^{-1} \\ &+ 2\|\alpha_{(N)} - \alpha_{(N)n(0)\ldots n(m-1)}\| \leqslant \epsilon.\end{aligned} \tag{2.25}$$

QED

Remark: Obviously this theorem can be generalized to a large class of non-polynomial extensive interactions and even beyond finite dimensional Lie algebras.

Theorem 2.2: Under the assumptions of Theorem 2.1 one has

$$\sup_{i,j,N} N\|[\alpha^i_{(N)}(s), \alpha^j_{(N)}(t)]\| < \infty \tag{2.26}$$

uniformly on compacts in s, t.

Proof: Starting from (2.19) one obtains

$$[A^i_{(N)}, \alpha^j_{(N)}(t)] = \sum_{k=1}^{l} C^{ij}_k \alpha^k_{(N)} + \sum_{k=1}^{l} \int_0^t dr \beta^{jk}(\underline{\alpha}_{(N)}(r), [A^i_{(N)}, \alpha^k_{(N)}(r)]), \tag{2.27}$$

where β^{jk} is linear in $[A^i_{(N)}, \alpha^k_{(N)}(r)]$. This linear Volterra equation can be solved by iteration, uniformly on compacts in t. By repeating this argument for

$$[A^i_{(N)}(s), \alpha^j_{(N)}(t)] = [A^i_{(N)}. \alpha^j_{(N)}(t)] + \sum_{k=1}^{l} \int_0^s dr \beta^{ik}(\underline{\alpha}_{(N)}(r), [A^k_{(N)}(r), \alpha^j_{(N)}(t)]) \tag{2.28}$$

with (2.27) as input, one obtains Theorem 2.2.

QED

The following theorem gives a classical interpretation to the time-evolution under extensive interaction for expectation values of intensive observables in classical states:

Theorem 2.3: Under the assumptions of Theorem 2.1, let ω be classical with respect

to $\mathscr{L}$ with probability measure μ_ω. Then ω is classical with respect to all intensive observables $\alpha^k_{(N)}(t)$, $1 \leqslant k \leqslant l$, $t \in \mathbf{R}$, and for all monomials

$$\lim_{N\to\infty} \omega(\alpha^i_{(N)}(r) \dots \alpha^j_{(N)}(t)) = \int \mu_\omega(d\underline{\gamma})\, \alpha^i(\underline{\gamma}, r) \dots \alpha^j(\underline{\gamma}, t) \tag{2.29}$$

uniformly on compacts in $r, \dots t$.

Here $\underline{\alpha}(\underline{\gamma}, t)$ is the solution of the ordinary differential equation

$$\begin{aligned} &\dot{\alpha}^k = \{\beta, \alpha^k\} = \beta^k(\underline{\alpha}), \\ &\alpha^k(\underline{\gamma}, 0) = \gamma^k, \end{aligned} \tag{2.30}$$

where β^k is obtained from $H_{(N)}$ by treating β as a polynomial in commuting variables $\alpha^1, \dots \alpha^l$ and by using the Poisson brackets $\{\alpha^i, \alpha^j\} = i \sum C^{ij}_k \alpha^k$.

In particular, if ω is pure with respect to $\alpha^1_{(N)}, \dots \alpha^l_{(N)}$, then ω is also pure with respect to all $\alpha^k_{(N)}(t)$.

Remark: In this framework, the classical limit (the limit $N \to \infty$) establishes the following correspondence:

Quantum-classical correspondence

Quantum mechanics	Classical mechanics
Classical state	Ensemble in phase space†
Pure classical state	Point in phase space
Intensive observable	Function on phase space
Heisenberg time evolution	Hamiltonian time evolution
$iN[\alpha^p_{(N)}, \alpha^q_{(N)}]$	$\{\alpha^p, \alpha^q\}$

Proof: If one can show that the classical equations

$$\alpha^k(t) = \alpha^k(s) + \int_s^t dr \beta^k(\underline{\alpha}(r)) \tag{2.31}$$

have iterative solutions $\alpha^k_{n(0)\dots n(m)}(t) \to \alpha^k(t)$ for $md \leqslant t \leqslant (m+1)d$, as in Theorem 2.1, then clearly (2.29) will hold. This is so, since every pair of finite approximations $\underline{\alpha}_{(N)\, n(0)\dots n(m)}(t)$ and $\underline{\alpha}_{n(0)\dots n(m)}(\underline{\gamma}, t)$ to the quantum and classical equations (the latter with initial condition $\underline{\gamma}$ at $t = 0$) satisfy

$$\begin{aligned} &\lim_{N\to\infty} \omega(\alpha^i_{(N)m(0)\dots m(\rho)}(r) \dots \alpha^j_{(N)n(0)\dots n(\tau)}(t)) \\ &\quad = \int \mu_\omega(d\underline{\gamma})\, \alpha^i_{m(0)\dots m(\rho)}(\underline{\gamma}, r) \dots \alpha^j_{n(0)\dots n(\tau)}(\underline{\gamma}, t), \end{aligned} \tag{2.32}$$

since ω is a classical state. The left-hand side of (2.32) approximates the left-hand side of (2.29) uniformly in N, by Theorem 2.1. By the iterative construction for (2.31), the integrand of the right-hand side of (2.32) is uniformly bounded by an integrable function and converges pointwise for $m(0), \dots m(\rho), \dots, n(0), \dots n(\tau) \to \infty$ to $\alpha^i(\underline{\gamma}, r) \dots$

† A phase space $\mathbf{R}^{2f}$ with the symplectic structure of classical Hamiltonian mechanics can be obtained by group contraction from $SU(2)^f$ (see the laser model in Section 5).

$\alpha^j(\underline{\gamma},t)$. Hence the right-hand side of (2.32) converges to the right-hand side of (2.29) by the dominated convergence theorem.

That the classical equations have global solutions follows from a group-theoretical argument: Complete $A^1, \ldots A^l$ to a real basis $A^1, \ldots A^L$ of the Lie algebra $\mathfrak{G}$ of $GL(K,\mathbf{C})$, $L = K^2$. $\mathfrak{G}$ has the Casimir operator

$$C = \sum_{i,j=1}^{K} E^{ij*} E^{ij} = \sum_{i,j=1}^{L} x_{ij} A^i A^j, \tag{2.33}$$

where (x_{ij}) is a positive definite $L \times L$ matrix. In the extended phase space $\mathbf{R}^L$ one can study the differential equation

$$\dot{\alpha}^i = \{\beta, \alpha^i\}, \quad 1 \leqslant i \leqslant L, \tag{2.34}$$

where the α^i correspond to the A^i and have well-defined Poisson brackets $\{\alpha^i, \alpha^j\}$ and where $\beta = \beta(\alpha^1, \ldots \alpha^i)$ is independent of $\alpha^{l+1}, \ldots \alpha^L$. For initial conditions $\alpha^i(\underline{\gamma},0) = \gamma^i$, $1 \leqslant i \leqslant l$, and $\alpha^i(\underline{\gamma},0) = 0$, $l+1 \leqslant i \leqslant L$, the $\alpha^i(\underline{\gamma},t)$, $1 \leqslant i \leqslant l$, are the solutions of (2.30). Since

$$\{\beta, \textstyle\sum x_{ij} \alpha^i \alpha^j\} = 0,$$

one has for all t

$$\sum_{i,j=1}^{L} x_{ij} \alpha^i(\underline{\gamma},t)\, \alpha^j(\underline{\gamma},t) = \sum_{i,j=1}^{l} x_{ij} \gamma^i \gamma^j. \tag{2.35}$$

Since (x_{ij}) is positive definite, the $\alpha^i(\underline{\gamma},t)$ stay bounded uniformly in t. Hence the iteration scheme can be used for all times in the classical equations (2.30).

QED

Theorem 2.4: Under the conditions of Theorem 2.1 let $\alpha^1_{(N)}, \ldots \alpha^l_{(N)}$ have normal fluctuations in ω around $\gamma^1, \ldots \gamma^l$. Then, for all times t and all $1 \leqslant k \leqslant l$, the $\alpha^k_{(N)}(t)$ have normal fluctuations in ω around $\alpha^k(\underline{\gamma},t)$, and for all monomials in

$$a^k_{(N)}(t) \equiv N^{1/2}(\alpha^k_{(N)}(t) - \alpha_k(\underline{\gamma},t))$$
$$\lim_{N\to\infty} \omega(a^i_{(N)}(r) \ldots a^j_{(N)}(t)) = (\Omega_\omega, a^i_\omega(r) \ldots a^j_\omega(t)\, \Omega_\omega). \tag{2.36}$$

Here, $a^k_\omega(t)$ is the solution of the linear variational equation of (2.30) around $\underline{\alpha}(\underline{\gamma},t)$ with initial condition $\alpha^k_\omega(0) = a^k_\omega$.

Proof: By taking the difference between (2.17) and (2.31) one obtains

$$a^k_{(N)}(t) = a^k_{(N)} + \int_0^t ds N^{1/2}(i[H_{(N)}(s), \alpha^k_{(N)}(s)] - \{\beta(x), \alpha^k(s)\}). \tag{2.37}$$

In the integrand of (2.37) we combine corresponding terms

$$N^{1/2}[\alpha^{k(1)}_{(N)}(s) \ldots \alpha^{k(m)}_{(N)}(s) - \alpha^{k(1)}(s) \ldots \alpha^{k(m)}(s)] = \sum_{\mu=1}^{m} a^{k(\mu)}(s) \prod_{\substack{\nu=1 \\ \nu\neq\mu}}^{m} \alpha^{k(\nu)}(s) + \sum_{k=1}^{l} \delta^k_{(N)}(s). \tag{2.38}$$

Each $\delta^k_{(N)}(s)$ is a sum of monomials (with coefficients independent of N) in $\alpha^i_{(N)}(s)$,

$\alpha^j(s)$, $1 \leqslant i, j \leqslant l$, and is linear in $a^k_{(N)}(s)$. $\delta^k_{(N)}(s)$ contains at least one factor of the type $(\alpha^j_{(N)}(s) - \alpha^j(s))$. We consider (2.37) as a linear Volterra equation for the $a^k_{(N)}(t)$. The iterative solution converges in the ω-expectation to (2.36), since, by Theorem 2.3, the $\delta^k_{(N)}$-terms do not contribute in the limit $N \to \infty$.

QED

It is clear that the above class of non-linear differential equations does not show self-oscillatory behaviour, since the equations of motion generated by the time independent Hamiltonian, β, have at least β and the Casimir functions of the Lie group as integrals of motion. In other words, a system with a globally attractive limit cycle would necessarily have $\beta =$ constant on that limit cycle, and this cannot be reached by an initial state with a different value of β, because β is a non-constant analytic function of the phase space coordinates. In the context of these models, 'coarse graining' does not give rise to irreversible behaviour. Hence, in order to build a system having laser-like behaviour, dissipation is an absolute necessity. We turn to that question in the next section.

3. Linear Dissipation in Fermi Systems

Having previously considered a system consisting of many small systems coupled together by a mean field like Hamiltonian (i.e. an interaction which does not distinguish the relative location of the small systems), we now introduce the concept of the reservoir. The small systems will be composed of fermions, and each small system will have its own reservoir which is taken to be a fermion field of infinitely many degrees of freedom. We shall begin by studying the one system–one reservoir pair. It is then easy to describe many such pairs simultaneously and to see how the law of large numbers determines the properties of the intensive and fluctuation observables.

The use of fermion reservoirs, instead of boson or two-level atom reservoirs, has a mathematical and a physical motivation. From the mathematical point of view, the simplicity of dealing with bounded operators is obvious, and it turns out that the equations of motion have a closed solution (this boundedness would not be true if one used the boson reservoir mentioned in the introduction [S1]). Physically, dissipation by fermion–fermion coupling can hold for superconductors and for atoms in a solid state laser. In both cases the small system fermions are really identifiable as electrons (cf. Section 5).

We first consider one fermion $a^\#$ coupled to two Fermi fields $A^\#_w$, $B^\#_w$, where the parameter w characterizes the degrees of freedom of the Fermi field, and w varies over $\mathbf{R}^1$ for simplicity. All operators anticommute except for

$$\{a, a^\#\} = 1, \quad \{A_w, A^*_{w'}\} = \{B_w, B^*_{w'}\} = \delta(w - w'). \tag{3.1}$$

Let $\mathscr{A}^F$ be the C^*-algebra generated by $a^\#$ and the smeared-out $A^\#_w$, $B^\#_w$. The Hamiltonian

$$H^0 = \int_{-\infty}^{+\infty} dw w (A^*_w A_w + B^*_w B_w) \tag{3.2}$$

is the infinitesimal generator (in the Fock representation) of the continuous 1-parameter group α^0_t of automorphisms of $\mathscr{A}^F$, which acts (in distribution language) as $a \to a$,

$C_w \to C_w \exp(-iwt)$. For simplicity, we shall often use the symbol C to stand either for A or for B. For $\epsilon > 0$

$$V_\varepsilon = \int dw\, e^{-\varepsilon w^2}\{(g_A^* A_w^* + g_B^* B_w^*)\, a + \text{h.c.}\} \tag{3.3}$$

belongs to $\mathscr{A}^F$. Hence $H = H^0 + V$ also generates a 1-parameter group α_t^ε of automorphisms of $\mathscr{A}^F$, and the action of α_t^ε can be computed by a norm-convergent Dyson series. The operators $a^\varepsilon(t) = \alpha_t^\varepsilon(a)$ and $C_w^\varepsilon(t) = \alpha_t^\varepsilon(C_w)$ are solutions of the linear Heisenberg equations

$$\begin{aligned} \dot{a}^\varepsilon(t) &= -i \int dw\, e^{-\varepsilon w^2}\{g_A A_w^\varepsilon(t) + g_B B_w^\varepsilon(t)\}, \\ \dot{C}_w^\varepsilon(t) &= -iwC_w^\varepsilon(t) - ig_C^* \exp(-\epsilon w^2)\, a^\varepsilon(t). \end{aligned} \tag{3.4}$$

Hence, one can express $C_w^\varepsilon(t)$ in terms of the initial condition C_w at $t = 0$ and by $a^\varepsilon(s)$ for $|s| \leqslant t$:

$$C_w^\varepsilon(t) = e^{-iwt} C_w - ig_C^* \int_0^t ds \exp - (\epsilon w^2 + iw(t-s))\, a^\varepsilon(s). \tag{3.5}$$

This leads to the linear Volterra equation

$$\begin{aligned} a^\varepsilon(t) = a &- (|g_A|^2 + |g_B|^2) \int_0^t ds a^\varepsilon(s)\, \delta^\varepsilon(t-s) \\ &- i \int_0^t ds \int dw\{g_A A_w + g_B B_w\} \exp -(\epsilon w^2 + iws). \end{aligned} \tag{3.6}$$

As $\epsilon \downarrow 0$, $\delta^\varepsilon(s) \to 2\pi\delta(s)$. One easily deduces from the iterative solution of (3.6):

Theorem 3.1: Let $\gamma = \pi(|g_A|^2 + |g_B|^2)$. Then for all $t \in \mathbf{R}^1$ and $h \in \mathscr{S}(\mathbf{R}^1)$

$$n - \lim_{\varepsilon \downarrow 0} a^\varepsilon(t) = a(t) = e^{-\gamma|t|}\, a - i \int_0^t ds\, e^{-\gamma|t-s|}\{g_A A(s) + g_B B(s)\}, \tag{3.7}$$

$$n - \lim_{\varepsilon \downarrow 0} \int dw h(w)\, C_w^\varepsilon(t) = \int dw h(w)\, C_w(t), \tag{3.8}$$

where

$$C(s) = \int dw\, C_w \exp(-iws), \tag{3.9}$$

$$C_w(t) = e^{-iwt} C_w - ig_C^* \int_0^t ds a(s) \exp - iw(t-s). \tag{3.10}$$

$(a, C_w) \leftrightarrow (a(t), C_w(t))$ can be extended to a strongly continuous 1-parameter group of automorphisms of $\mathscr{A}^F$, $\alpha_t(A) = n - \lim \alpha_t^\varepsilon(A)$.

Comment: When $\epsilon > 0$, the reservoir, as defined by $H^0 + V_\epsilon$, is called regular. By modifying H^0 (e.g. $w \to (w^2+1)^{1/2}$), one could even make the energy bounded from below. The equation (3.6) can be solved by Laplace transform. We shall return to the study of regular reservoirs in a later paper.

In the sequel we shall always take $t \geqslant 0$. Then $a(t)$ is the solution of the differential equation

$$\dot{a}(t) = -\gamma a(t) - ig_A A(t) - ig_B B(t) \tag{3.11}$$

with 'damping constant' $\gamma \geqslant 0$ and 'fluctuation force' $F(t) = -ig_A A(t) - ig_B B(t)$. The Hilbert space of the system $a^\#$ and the reservoir $A_w^\#$, $B_w^\#$ will be taken as $\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_R$. The initial state ω at $t = 0$ of the combined system has to describe the coupling of the system in any state ω_S (an arbitrary density matrix in $\mathscr{H}_S \simeq \mathbf{C}^2$) to the reservoir in the state ω_R, which is 'full' of B-quanta and 'empty' of A-quanta. Hence we take $\omega = \omega_S \otimes \omega_R$, with $\omega_R = (\Omega_R, \cdot\, \Omega_R)$, i.e. the vector state Ω_R in the Fock space $\mathscr{H}_R$ which satisfies

$$A_w \Omega_R = B_w^* \Omega_R = 0, \quad \forall\, w \in \mathbf{R}. \tag{3.12}$$

The $A^\#(t)$ and $B^\#(t)$ act like 'white noise': they are 'Gaussian' in the sense that all truncated ω_R-expectations of order >2 vanish. They are also 'Markovian' and stationary with zero mean, since the only non-vanishing ω_R-expectations of order $\leqslant 2$ are

$$\omega_R(A(s)\, A^*(t)) = \omega_R(B^*(s)\, B(t)) = 2\pi\delta(s-t). \tag{3.13}$$

One deduces from (3.7) and (3.13) that the following limits are attained with errors that vanish exponentially in time:

$$\begin{aligned} &\lim_{t\to+\infty} \omega(a^\#(t)) = 0 \\ &\lim_{t\to+\infty} \omega(a^*(t)\, a(t)) = |g_B|^2 (|g_A|^2 + |g_B|^2)^{-1}. \end{aligned} \tag{3.14}$$

Let $\omega_S(t)$ be the partial expectation over ω_R of $\omega = \omega_S \otimes \omega_R$ evolved under α_t. By (3.14), $\omega_S(t)$ converges to the Gibbs state for $a^* a$ with a temperature $(kT)^{-1} = \ln|g_A|^2 - \ln|g_B|^2 \in (-\infty, \infty)$.

From Theorem 3.1, the anticommutation relations between $a^\#(r)$, $C_w^\#(s)$ and $C^\#(t)$ follow for all times. For instance,

$$\begin{aligned} &\{a(s), a^*(t)\} = \exp -\gamma|t-s|, \\ &\{A(t), a^*(t)\} = i\pi g_A^*, \\ &\{B(t), a^*(t)\} = i\pi g_B^*, \\ &\{C(t), a(t)\} = 0. \end{aligned} \tag{3.15}$$

(3.15) is not in contradiction with the distribution identity $\{A(t), a^*(0)\} = 0$ for all t. One has to be careful in computations in the singular reservoir. Ambiguities are resolved by taking limits after a regularization: $a(t) = \lim a^\epsilon(t)$.

The above formalism of linear dissipation will now be generalized to a 'small' system of infinitely many fermions, each coupled to its private big reservoir. In the spirit of Section 2, we have a countable number of C^*-algebras $\mathscr{A}_n^F$, $n \in \mathbf{Z}$, each of which is generated by M Fermi operators $a_n^{m\#}$, $1 \leqslant m \leqslant M$, with their own reservoir operators $A_{nw}^{m\#}$, $B_{nw}^{m\#}$. For all $1 \leqslant m \leqslant M$, $n \in \mathbf{Z}$, we assume

$$\{a_n^m, a_n^{m*}\} = 1,$$
$$\{A_{nw}^m, A_{nw'}^{m*}\} = \{B_{nw}^m, B_{nw'}^{m*}\} = \delta(w - w') \tag{3.16}$$

and that all other anticommutators between first degree fermion operators vanish. $\mathscr{A}_n^F$ contains the quasilocal C^*-algebra $\mathscr{A}_n$, generated by all particle-conserving fermion polynomials at site n. $\mathscr{A}_n$ contains the operators

$$S_n^{kl} = a_m^{k*} a_n^l, \quad 1 \leqslant k, l \leqslant M, \tag{3.17}$$

which are a basis of the Lie algebra $\mathscr{L} = \mathrm{Lie}\, U(M)$ of $U(M)$. By taking instead of $\mathscr{A}_n$ the *even* fermion algebra $\mathscr{A}_n^e \subset \mathscr{A}_n^F$, we could have included operators of the type $(a_n^k a_n^l)^*$ and obtain the Lie algebra of $O(2M)$. Since all our examples are inbedded in $\mathrm{Lie}\, U(M)$, we refrain from this notational complication.

For finitely many sites, $1 \leqslant n \leqslant N$, we shall consider the linear dissipation described by the Hamiltonian

$$H_{(N)}^R = \sum_{n=1}^{N} H_n^R,$$
$$H_n^R = \sum_{m=1}^{M} \left\{ \int dw (A_{nw}^{m*} A_{nw}^m + B_{nw}^{m*} B_{nw}^m)\, w + \int dw (g_A^{m*} A_{nw}^{m*} a_n^m + g_B^{m*} B_{nw}^{m*} a_n^m + \text{h.c.}) \right\}, \tag{3.18}$$

where we assume

$$\gamma^m \equiv \pi(|g_A^m|^2 + |g_B^m|^2) > 0 \quad \text{for all } 1 \leqslant m \leqslant M.$$

With

$$C_n^m(t) = \int dw C_{nw}^m \exp(-iwt) \tag{3.19}$$

the time evolution of the local fermion operators, $a_n^m(t)$, is again of the type (3.11). Using (3.15), the resulting differential equations for the

$$S_n^{kl}(t) = \exp(iH_n^R t)\, S_n^{kl} \exp(-iH_n^R t) \quad \text{for } t \geqslant 0$$

become

$$S_n^{kl}(t) = \delta^{kl} \eta^k - \gamma^{kl} S_n^{kl}(t) + F_{n+}^{kl}(t) + F_{n-}^{kl}(t), \tag{3.20}$$

where δ^{kl} is the Kronecker delta and

$$\eta^k = 2\pi |g_B^k|^2, \quad \gamma^{kl} = \gamma^k + \gamma^l,$$
$$F_{n+}^{kl}(t) = i g_A^{k*} A_n^k(t)^* a_n^l(t) + i g_B^l B_n^l(t)\, a_n^k(t)^*,$$
$$F_{n-}^{kl}(t) = -i g_B^{k*} a_n^l(t)\, B_n^k(t)^* - i g_A^l a_n^k(t)^* A_n^l(t). \tag{3.21}$$

The separation (3.20) into damping constants γ^{kl}, pump parameters η^k, and fluctuation forces $F_{n\pm}^{kl}(t)$ is natural, if one considers states $\omega = \omega_S \otimes \omega_R$ in which the reservoir $\omega_R = (\Omega_R, \cdot\, \Omega_R)$ is full of B-quanta and empty of A-quanta:

$$A_{nw}^m \Omega_R = B_{nw}^{m*} \Omega_R = 0 \tag{3.22}$$

for all m, n, w. It follows from (3.21) that, however complicated the $a_n^{m}(t)^{\#}$ may be (and they will be complicated in the next section), the partial trace

$$\omega_R(F_{n\pm}^{kl}(t)) = 0,$$

since

$$F_{n-}^{kl}(t)\,\Omega_R = F_{n+}^{kl}(t)^*\,\Omega_R = 0. \tag{3.23}$$

The fact that every local fermion operator $a_n^{m\#}$ is coupled to its own reservoir implies a strong law of large numbers for the M^2 intensive observables (which we collectively write in vector notation as $\underline{\sigma}_{(N)}$),

$$\sigma_{(N)}^{kl}(t) = N^{-1}\sum_{n=1}^{N} S_n^{kl}(t), \tag{3.24}$$

under the time evolution $H_{(N)}^{R}$:

Theorem 3.2: Assume that ω has the form $\omega_S \otimes \omega_R$, where ω_R satisfies (3.22) and ω_S is classical with respect to $\underline{\sigma}_{(N)}$ with probability measure μ_ω. Then ω is classical with respect to $\underline{\sigma}_{(N)}(t)$ and for all monomials

$$\lim_{N\to\infty} \omega(\sigma_{(N)}^{ij}(t)\ldots\sigma_{(N)}^{pq}(s)) = \int \mu_\omega(d\underline{\alpha})\,\sigma^{ij}(\underline{\alpha},t)\ldots\sigma^{pq}(\underline{\alpha},s) \tag{3.25}$$

uniformly on compacts in $t, \ldots s$. For all $t \in \mathbf{R}$, $\underline{\sigma}(\underline{\alpha},t)$ is the solution of the linear dissipative equation

$$\begin{aligned}&\dot{\sigma}^{kl}(\underline{\alpha},t) = \delta^{kl}\eta^k - \operatorname{sgn}(t)\,\gamma^{kl}\,\sigma^{kl}(\underline{\alpha},t),\\ &\underline{\sigma}(\underline{\alpha},0) = \underline{\alpha},\end{aligned} \tag{3.26}$$

i.e.

$$\sigma^{kl}(\underline{\alpha},t) = \exp(-\gamma^{kl}|t|)\,\alpha^{kl} + \delta^{kl}[\eta^k - \exp(-\gamma^{kl}|t|)]/\gamma^{kl}. \tag{3.27}$$

Proof: From (3.20) one obtains for $t \geqslant 0$:

$$\dot{\sigma}_{(N)}^{kl}(t) = \delta^{kl}\eta^k - \gamma^{kl}\,\sigma_{(N)}^{kl}(t) + \varphi_{(N)}^{kl}(t), \tag{3.28}$$

where

$$\varphi_{(N)}^{kl}(t) = \varphi_{(N)+}^{kl}(t) + \varphi_{(N)-}^{kl}(t),$$

and

$$\varphi_{(N)\pm}^{kl}(t) = N^{-1}\sum_{n=1}^{N} F_{n\pm}^{kl}(t). \tag{3.29}$$

Hence,

$$\sigma_{(N)}^{kl}(t) = \sigma_{(N)}^{kl}\exp(-\gamma^{kl}t) + \delta^{kl}[\eta^k - \exp(-\gamma^{kl}t)]/\gamma^{kl} + \hat{\sigma}_{(N)}^{kl}(t). \tag{3.30}$$

Here,

$$\hat{\sigma}_{(N)}^{kl}(t) = \int_0^t ds \exp -\gamma^{kl}(t-s)\,\varphi_{(N)}^{kl}(s) \tag{3.31}$$

is explicitly known, using the solution (3.7) for the $a_n^m(s)^{\#}$ occurring in $\varphi_{(N)}^{kl}(s)$. One obtains (3.27), if one can show that, for all $r, \ldots t$ and all monomials (with $i = (i_1, i_2)$, $1 \leqslant i\rho \leqslant M$),

$$\lim_{N\to\infty} \omega(\sigma_{(N)}^{i} \ldots \sigma_{(N)}^{j}\, \hat{\sigma}_{(N)}^{k}(r) \ldots \hat{\sigma}_{(N)}^{l}(t)\, \sigma_{(N)}^{m} \ldots \sigma_{(N)}^{n}) = 0. \tag{3.32}$$

Since

$$\hat{\sigma}_{(N)}^{k}(r) = \hat{\sigma}_{(N)+}^{k}(r) + \hat{\sigma}_{(N)-}^{k}(r),$$

where the first term annihilates ω on the left- and the second on the right-hand side, it suffices to show that

$$[\sigma_{(N)}^{j}, \hat{\sigma}_{(N)\pm}^{k}(t)] = O(N^{-1}), \tag{3.33}$$

$$[\hat{\sigma}_{(N)\pm}^{j}(s), \hat{\sigma}_{(N)\pm}^{k}(t)] = O(N^{-1}) \tag{3.34}$$

for $N \to \infty$. To prove this we use (3.15) and (3.21):

$$[\sigma_{(N)}^{kl}, \hat{\sigma}_{(N)+}^{pq}(t)] = -\frac{i}{N^2} \sum_{n=1}^{N} \int_0^t ds \exp -\gamma^{pq}(t-s) \times \{g_A^{p*} A_n^p(s)^* a_n^l \delta^{kq} \exp(-\gamma^q s) - g_B^q B_n^q(s)\, a_n^{k*} \delta^{lp} \exp(-\gamma^p s)\}. \tag{3.35}$$

Since the smeared-out A- and B-fields are bounded operators, (3.33) is manifestly $O(N^{-1})$. In the $(-,+)$-case, which is the most interesting, (3.34) leads to the majorization of

$$[\varphi_{(N)-}^{kl}(s), \varphi_{(N)+}^{pq}(t)] = N^{-2} \sum_{n=1}^{N} [(g_B^{k*} a_n^l(s)\, B_n^k(s)^* + g_A^l a_n^k(s)^* A_n^l(s)), (g_A^{p*} A_n^p(t)^* a_n^q(t) + g_B^q B_n^q(t)\, a_n^p(t)^*]. \tag{3.36}$$

(3.36) can be evaluated in terms of anticommutators, by using the identity

$$[UV, XY] = U\{V, X\}Y - \{U, X\}\{V, Y\} + XU\{V, Y\} + \{U, X\}YV - X\{U, Y\}V, \tag{3.37}$$

and one obtains

$$N^{-2} \sum_{n=1}^{N} [2\pi |g_B^k|^2 \delta^{kq} \delta(s-t)\, a_n^l(s)\, a_n^p(s)^* + 2\pi |g_A^l|^2 g^{lp} \delta(s-t)\, a_n^k(s)^* a_n^q(s) - g_B^{k*} g_A^{p*} \{a_n^l(s), A_n^p(t)^*\}\{B_n^k(s)^*, a_n^q(t)\} \tag{3.38}$$

and similar terms of the type $\{U, X\}\{V, Y\}$

$$+ g_B^{k*} g_B^q B_n^q(t)\, a_n^l(s) \{B_n^k(s)^*, a_n^p(t)^*\}$$

and similar terms with either B or A^* to the left or B^* or A to the right.

The first two terms are $O(N^{-1})$, when integrated over s and t. From (3.7), one obtains

$$\{a_n^l(s), A_n^p(t)^*\} = -2\pi i g_A^l \delta^{lp} \theta(s-t) \exp -\gamma^l(s-t). \tag{3.39}$$

Hence the third term is $O(N^{-1})$ and has support in $\{s = t\}$, and can therefore be omitted under the s–t-integration. All other terms are $O(N^{-1})$ and annihilate ω either to the left- or to the right-hand side. The commutators of the type $[\varphi^{kl}_{(N)-}(s), \varphi^{pq}_{(N)-}(t)]$ are of similar structure, except that the $\delta(s-t)$-terms are missing.

QED

(3.35) and (3.38) are useful in the following investigation up to $o(1)$ of the commutators of fluctuation observables, which are larger by a factor N:

Theorem 3.3: Under the assumption of Theorem 3.2, let $\underline{\sigma}_{(N)}$ have normal fluctuations in ω_S around $\underline{\alpha}$. Then the $\underline{\sigma}_{(N)}(t)$ have normal fluctuations in ω around $\underline{\sigma}(\underline{\alpha}, t)$ (cf. (3.26)), and the limits $s(t)$ of the fluctuation observables

$$\sqrt{N}(\underline{\sigma}_{(N)}(t) - \underline{\sigma}(\underline{\alpha}, t)) = \underline{s}_{(N)}(t),$$

$$\lim_{N\to\infty} \omega(s^{ij}_{(N)}(r) \ldots s^{pq}_{(N)}(t)) = (\Omega, s^{ij}(r) \ldots s^{pq}(t)\,\Omega),$$

are solutions of the linear inhomogeneous equations ($t \geqslant 0$):

$$\dot{s}^{kl}(t) = -\gamma^{kl} s^{kl}(t) + f^{kl}_{\omega}(t),$$
$$s^{kl}(0) = s^{kl}_{\omega}, \tag{3.40}$$

where the fluctuation forces $f^{kl}_{\omega}(t)$ will be defined by (3.45).

Proof: For $t \geqslant 0$, $\underline{s}_{(N)}(t)$ can be evaluated from (3.30) and (3.27):

$$s^{kl}_{(N)}(t) = s^{kl}_{(N)} \exp[-\gamma^{kl} t] + \int_0^t ds f^{kl}_{(N)}(s) \exp[-\gamma^{kl}(t-s)], \tag{3.41}$$

where $\underline{f}_{(N)}(s) = \sqrt{N}\,\underline{\varphi}_{(N)}(s)$. Instead of (3.32) we have now to investigate the limit $N \to \infty$ of

$$\omega(s^{i}_{(N)} \ldots s^{j}_{(N)} f^{k}_{(N)}(r) \ldots f^{l}_{(N)}(t)\, s^{m}_{(N)} \ldots s^{n}_{(N)}). \tag{3.42}$$

Now, $[s^{kl}_{(N)}, f^{pq}_{(N)+}(t)]$ leads to N times the integrand of (3.35) and, when integrated over t, is $O(1)$ for $N \to \infty$. However, this commutator is a sum of two terms which annihilate ω either to the left- or to the right-hand side. The commutator of this commutator with $s^{xy}_{(N)}$ or $f^{xy}_{(N)}(r)$ is $O(N^{-1/2})$, by the same argument. Hence $[s^{kl}_{(N)}, f^{pq}_{(N)}(t)]$ can be dropped in (3.42) for $N \to \infty$.

Similarly, $[f^{kl}_{(N)-}(s), f^{pq}_{(N)+}(t)]$ is $O(1)$, when integrated over s and t. Here N times the first two terms in (3.38) converge in (3.42) to the c-numbers

$$\Delta^{kl,\,pq}(s,t) \equiv 2\pi\delta(s-t)\{\delta^{kq}\,\delta^{lp}|g^{k}_{B}|^2 - \delta^{kq}\,\sigma^{pl}(\alpha,t)|g^{k}_{B}|^2 + \delta^{lp}\,\sigma^{kq}(\underline{\alpha},t)|g^{l}_{A}|^2\}. \tag{3.43}$$

The $\{U,X\}\{V,Y\}$-terms vanish when integrated over s and t. The others have $O(N^{-1/2})$ commutators with $s^{xy}_{(N)}$ and $f^{xy}_{(N)}(r)$ and annihilate ω either to the left- or to the right-hand side. Hence they can be dropped for $N \to \infty$.

Thus the limit $N \to \infty$ of (3.42) has the form

$$(\Omega_S, s^{i}_{\omega} \ldots s^{n}_{\omega}\,\Omega_S)(\Omega_R, f^{k}_{\omega}(r) \ldots f^{l}_{\omega}(t)\,\Omega_R), \tag{3.44}$$

where the operators s^{i}_{ω} and $f^{k}_{\omega}(r)$ act in different Hilbert spaces $\mathscr{H}_S$ and $\mathscr{H}_R$. $\mathscr{H}_S$, with

vacuum Ω_S, is the Hilbert space of the GNS construction for the fluctuation operators s^i_ω at $t=0$ (cf. (2.7)). The $f^{kl}_\omega(s) = f^{kl}_{\omega+}(s) + f^{kl}_{\omega-}(s)$ are generalized Bose fields in a Fock space $\mathscr{H}_R$ with vacuum Ω_R satisfying for all s, t and all k, l, p, q:

$$f^{kl}_{\omega-}(s)\,\Omega_R = 0 = f^{kl}_{\omega+}(s)^*\,\Omega_R,$$
$$[f^{kl}_{\omega-}(s), f^{pq}_{\omega-}(t)] = 0,$$
$$[f^{kl}_{\omega-}(s), f^{pq}_{\omega+}(t)] = \Delta^{kl,\,pq}(s,t). \tag{3.45}$$

Hence we obtain (3.40). To the damping of the fluctuations, γ^{kl}, the dissipation adds a fluctuation force $f^{kl}_{(N)}(t)$, which does not vanish for $N \to \infty$. However, from the messy expression for finite N, $f^{kl}_{(N)}(t)$ is 'purified' by the law of large numbers to a Gaussian and Markovian external force, $f^{kl}_\omega(t)$. For $t \to \infty$, the $f^{kl}_\omega(t)$ become stationary and independent of ω, since

$$\Delta^{kl,\,pq}(s,t) \to 2\pi\delta(s-t)\,\delta^{kp}\,\delta^{lp}|g^k_B|^2. \tag{3.46}$$

QED

Remark: (1) If the model is changed so that all fermions $a^{m\#}_n$ are coupled to one and the same reservoir, then the macroscopic equations are drastically changed even in $O(N)$, and they no longer lead to the phenomenologically accepted exponential decay law (3.27).

(2) The limits $\epsilon \downarrow 0$ (from a regular to a singular reservoir) and $N \to \infty$ can be interchanged in Theorems 3.2 and 3.3.

4. Fermi Systems with Mean Field Interaction and Linear Dissipation

Now we shall combine the structures of Section 2 and 3. The main result will be that for $N \to \infty$ the intensive observables obey ordinary differential equations which are the sum of a Hamiltonian and a linear dissipative part. In a normally fluctuating state, the fluctuations around the expectation values of the intensive observables obey linearized equations with a Gaussian and Markovian external force. These fluctuation forces are Bose fields in a Fock representation with commutators determined by the instantaneous values of the intensive observables.

As in Section 3, the building blocks of the dynamics are fermions $a^{m\#}_n$ with reservoirs $A^{m\#}_{nw}$, $B^{m\#}_{nw}$ and the Lie algebra is Lie $U(M)$. As Hamiltonian for the finite system ($N < \infty$) we take

$$H_{(N)} = H^S_{(N)} + H^R_{(N)}. \tag{4.1}$$

$H^S_{(N)} = N\beta(\underline{\sigma}_{(N)})$ is a self-adjoint extensive polynomial, and $H^R_{(N)}$ has the form (3.18). $H^S_{(N)} \in \mathscr{A}$ can be considered to be a perturbation of the $H^R_{(N)}$-automorphism group of Theorem 3.1. Therefore $H_{(N)}$, too, determines a strongly continuous 1-parameter group of automorphisms $\alpha^t_{(N)}$ of $\mathscr{A}$.

For $t \geqslant 0$, the equations of motion for the local fermion operators $a^m_{n(N)}(t) = \alpha^t_{(N)}(a^m_n)$ are

$$\dot{a}^m_{n(N)}(t) = -\gamma^m\,a^m_{n(N)}(t) - ig^m_A\,A^m_n(t) - ig^m_B\,B^m_n(t) + i[H^S_{(N)}(t), a^m_{n(N)}(t)]. \tag{4.2}$$

The intensive observables satisfy

$$\dot{\sigma}^{kl}_{(N)}(t) = \delta^{kl}\,\eta^k - \gamma^{kl}\,\sigma^{kl}_{(N)}(t) + \varphi^{kl}_{(N)}(t) + i[H^S_{(N)}(t), \sigma^{kl}_{(N)}(t)]. \tag{4.3}$$

By the Lie structure, $i[H^S_{(N)}(t), \sigma^{kl}_{(N)}(t)]$ is a polynomial in $\underline{\sigma}_{(N)}(t)$. The fluctuation forces $\varphi^{kl}_{(N)}(t)$ have the form (3.21), (3.29) with $a^m_{n(N)}(t)$ replaced by the very complicated solution $a^m_{n(N)}(t)$ of the local equations (4.2). However, if we consider initial states at $t=0$ of the type $\omega = \omega_S \otimes \omega_R$ with $\omega_R = (\Omega_R, \cdot \Omega_R)$ satisfying (3.22), one still has

$$\varphi^{kl}_{(N)}(t) = \varphi^{kl}_{(N)+}(t) + \varphi^{kl}_{(N)-}(t),$$
$$\varphi^{kl}_{(N)-}(t)\,\Omega_R = \varphi^{kl}_{(N)+}(t)^* \Omega_R = 0. \tag{4.4}$$

$\sum_{m=1}^M \sigma^{mm}_{(N)}(t)$ commutes with $H^S_{(N)}$. For suitable dissipations and special $H^S_{(N)}$, the equations of motion might fortuitously close on a subgroup of $U(M)$ (e.g. on $SU(2) \times SU(2)$). In this section we shall disregard this possibility, which will be discussed in the examples of Section 5.

As in Section 3, the direct integration of the equations of motion of the intensive observables,

$$\sigma^{kl}_{(N)}(t) = \sigma^{kl}_{(N)}(s) \exp[-\gamma^{kl}(t-s)] + \delta^{kl}(\eta^k - \exp[-\gamma^{kl}(t-s)]/\gamma^{kl}$$
$$+ \int_s^t dr \exp[-\gamma^{kl}(t-r)]\{i[H^S_{(N)}(r), \sigma^{kl}_{(N)}(r)] + \varphi^{kl}_{(N)}(r)\} \tag{4.5}$$

can be effected with only a qualitative knowledge of the $\varphi^{kl}_{(N)}(r)$, which depend on the local operators $a^m_{n(N)}(r)$:

Theorem 4.1: Let $\omega = \omega_S \otimes \omega_R$, where ω_S is classical with respect to $\underline{\sigma}_{(N)}$ with probability measure μ_ω, and ω_R satisfies (3.22). Then for all monomials

$$\lim_{N\to\infty} \omega(\sigma^{ik}_{(N)}(r) \ldots \sigma^{pq}_{(N)}(t)) = \int \mu_\omega(d\underline{\alpha})\, \sigma^{ik}(\underline{\alpha}, r) \ldots \sigma^{pq}(\underline{\alpha}, t) \tag{4.6}$$

uniformly on compacts in $r, \ldots t$. Here $\underline{\sigma}(\underline{\alpha}, t)$ is the solution of the classical equation

$$\dot{\sigma}^{kl} = \delta^{kl}\eta^k - \gamma^{kl}\sigma^{kl} + \{\beta, \sigma^{kl}\} \tag{4.7}$$

with $\underline{\sigma}(\underline{\alpha}, 0) = \underline{\alpha}$. In particular, if ω_S is pure with respect to $\underline{\sigma}_{(N)}$, then ω is a pure classical state with respect to all $\underline{\sigma}_{(N)}(t)$.

Proof: We first remark that the classical equations (4.7) have global solutions for every initial condition $\underline{\alpha} \in \mathbf{R}^{M^2}$: The Casimir function $\tau = \sum_{i,j=1}^M |\sigma^{ij}|^2$ of $U(M)$ satisfies $\{\beta, \tau\} = 0$, and therefore along every integral curve of (4.7)

$$\dot{\tau} = -\sum_{i,j=1}^M 2\gamma^{ij}|\sigma^{ij}|^2 + \sum_{k=1}^M 2\eta^k \sigma^{kk}. \tag{4.8}$$

Hence $\dot{\tau} = 0$ on the compact surface $\sum$ given by

$$\sum_{i\neq j} \gamma^{ij}|\sigma^{ij}|^2 + \sum_k \gamma^{kk}(\sigma^{kk} - \eta^k/2\gamma^{kk})^2 = \sum_k (\eta^k)^2(4\gamma^{kk})^{-1}. \tag{4.9}$$

Here we use the assumption on (3.18) that $\gamma^m > 0$ for all $1 \leqslant m \leqslant M$. Hence for all ρ sufficiently large, the regions $D_\rho = \{\sigma | \sum |\sigma^{ij}|^2 \leqslant \rho\}$ are invariant under the flow of (4.7), since $\dot{\tau} \leqslant 0$ on the boundary of D_ρ.

As in the proof of Theorem 2.2 we shall show that the quantum equations (4.5)

again have the fixed point property, that one can approximate $\underline{\sigma}_{(N)}(t)$ by $\underline{\sigma}_{(N)n(0)\ldots n(r)}(t)$ uniformly in N and that the ω-expectation values of the iterative solutions $\underline{\sigma}_{(N)n(0)\ldots n(r)}(t)$ converge to the μ_ω-mean of the corresponding classical approximations $\underline{\sigma}_{n(0)\ldots n(r)}(\underline{\alpha}, t)$.

By solving (4.5) for $\varphi^{kl}_{(N)}(r)$ and using the fact that $\|\sigma^{kl}_{(N)}(r)\| = 1$ uniformly in N, one proves that

$$\left\| \int_s^t dr \varphi^{kl}_{(N)}(r) \exp -\gamma^{kl}(t-r) \right\| \leqslant \text{const}\,(1 + |t-s|) \tag{4.10}$$

uniformly in N. Hence (4.5) again has the fixed point property, and the solution can be approximated uniformly in N by polynomials in the initial conditions $\underline{\sigma}_{(N)}$ (having the same structure as the approximating polynomials for the classical equations) and by integrals over the fluctuation forces $\varphi_{(N)}(s)$. We have to show that in every fixed order in the iteration scheme the fluctuation forces give a vanishing contribution in the ω-expectation

$$\omega(\sigma^i_{(N)} \ldots \sigma^j_{(N)} \varphi^k_{(N)}(r) \ldots \varphi^l_{(N)}(t)\, \sigma^m_{(N)} \ldots \sigma^n_{(N)}) \tag{4.11}$$

for $N \to \infty$. Using (4.4) this follows if one can commute the $\varphi^k_{(N)\pm}(r)$ freely among themselves and with the $\sigma^j_{(N)}$, with $O(N^{-1})$ errors for $N \to \infty$ when integrated over r.

For this purpose we investigate the behaviour of the anticommutators $\{a^m_{n(N)}(t)^\#, C^p_q(s)^\#\}$ for $N \to \infty$. For definiteness we consider

$$\{a^m_{n(N)}(t)^\#, A^1_1(s)^*\} \exp \gamma^m t \equiv b^m_{n(N)}(s,t)^\#. \tag{4.12}$$

We define $b^1 \equiv b^1_1$, $b^2 \equiv b^1_1{}^*$, ..., $b^{2M} \equiv b^M_1{}^*$, ... $b^{2MN} \equiv b^M_N{}^*$. Then the local equations (4.2) lead to the following linear Volterra equation for the anticommutators (4.12):

$$b^1_{(N)}(s,t) = -2\pi i g^1_A\, \theta(t-s) \exp \gamma^1 s + \int_0^t dr \left\{ \sum_{k=1}^{2M} P^{1k}_{(N)}(s,r) + N^{-1} \sum_{k=2M+1}^{2NM} P^{1k}_{(N)}(s,r) \right\}, \tag{4.13}$$

$$b^l_{(N)}(s,t) = \int_0^t dr \left\{ \sum_{k=2M(L-1)+1}^{2ML} P^{lk}_{(N)}(s,r) + N^{-1} \sum_{\substack{k=1 \\ k \notin [2M(L-1),\, 2ML]}}^{2MN} P^{lk}_{(N)}(s,r) \right\},$$

$(l > 1)$

where L satisfies $2M(L-1) < l \leqslant 2ML$ and where the $P^{lk}_{(N)}(s,r)$ are fixed polynomials in the local and intensive observables and linear in $b^k_{(N)}(s,r)$ with coefficients which are uniformly bounded in N. Hence one can 'compute' the $b^k_{(N)}(s,t)$ by iterating (4.13), and this series converges uniformly in N, since the $a^m_{n(N)}(r)^\#$ and $\underline{\sigma}_{(N)}(r)$ are uniformly bounded. Since the input vanishes for $s > t$, $b^k_{(N)}(s,t) \equiv 0$ for $s > t$. For $0 \leqslant s \leqslant t$, $b^k_{(N)}(s,t)$ is norm continuous in s, t and satisfies

$$\begin{aligned} &\sup_N \|b^k_{(N)}(s,t)\| < \infty, \quad 1 \leqslant k \leqslant 2M, \\ &\sup_N N\|b^k_{(N)}(s,t)\| < \infty, \quad 2M+1 \leqslant k \leqslant 2MN, \end{aligned} \tag{4.14}$$

uniformly in N and uniformly on compacts in t. By a similar system of linear Volterra equations one obtains for $N \to \infty$

$$\sup_{n,N} \|\{a^m_{n(N)}(t)^*, a^p_{n(N)}(s)^*\}\| < \infty$$

$$\sup_{n \neq q, N} N\|\{a^m_{n(N)}(t)^*, a^p_{q(N)}(s)^*\}\| < \infty, \tag{4.15}$$

uniformly on compacts in s, t, and hence

$$[\sigma^{kl}_{(N)}(s), \sigma^{pq}_{(N)}(t)] = O(N^{-1}). \tag{4.16}$$

Now the proof of Theorem 3.2 can be repeated, with the only difference being that the mean field interaction contributes $O(N^{-1})$ to the non-diagonal part in the anti-commutators, as shown in the second line of (4.15). Formerly this part vanished.

QED

Similarly, the limit of the fluctuation observables in a normally fluctuating state can be discussed by generalizing Theorems 2.4 and 3.3. Let $\mathscr{H}_S$ be the GNS Hilbert space of the fluctuation operators s^{kl} at time zero with cyclic vector Ω_S. Let $\mathscr{H}_R$ with vacuum Ω_R be the GNS Hilbert space of field operators $f^{kl}(s) = f^{kl}_+(s) + f^{kl}_-(s)$ satisfying (3.45) with $\Delta^{kl,pq}(s,t)$ of the form (3.43), where $\sigma^{kl}(\underline{\alpha}, t)$ are the solutions of the classical equations (4.7).

Theorem 4.2: Under the assumptions of Theorem 4.1 let $\underline{\sigma}_{(N)}$ have normal fluctuations in ω_S around $\underline{\alpha}$. Then all $s^{ik}_{(N)}(t) = N^{1/2}(\sigma^{ik}_{(N)}(t) - \sigma^{ik}(\underline{\alpha}, t))$ have normal fluctuations in $\omega = \omega_S \otimes \omega_R$. For every monomial

$$\lim_{N\to\infty} \omega(s^{ik}_{(N)}(r) \ldots s^{pq}_{(N)}(t)) = (\Omega, s^{ik}(r) \ldots s^{pq}(t)\, \Omega), \tag{4.17}$$

where $s^{ik}(t)$ is the solution (in $\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_R$ with vacuum $\Omega = \Omega_S \otimes \Omega_R$) of the linearized equations of (4.7) around $\sigma^{ik}(\underline{\alpha}, t)$ with inhomogeneity $f^{ik}(t)$.

Remark: The $f^{ik}(t)$ are Gaussian and Markovian, but not stationary, unless $\underline{\sigma}(\underline{\alpha}, t)$ is stationary.

Proof: By subtracting the quantum mechanical and the classical equations one obtains

$$s^{ik}_{(N)}(t) = s^{ik}_{(N)} \exp(-\gamma^{ik} t) + \int_0^t ds f^{ik}_{(N)}(s) \exp(-\gamma^{ik}(t-s))$$

$$+ \int_0^t ds\, N^{1/2} (i[H^S_{(N)}(s), \sigma^{ik}_{(N)}(s)] - \{\beta, \sigma^{ik}\}(s)) \exp(-\gamma^{ik}(t-s)). \tag{4.18}$$

As in Theorem 2.4, $N^{1/2}(i[H^S_{(N)}, \sigma^{ik}_{(N)}] - \{\beta, \sigma^{ik}\})(s)$ can be expressed in terms of polynomials in intensive observables $\underline{\sigma}_{(N)}(s)$ and classical solutions $\underline{\sigma}(s)$. Moreover, it

contains the $\underline{s}_{(N)}(s)$ linearly. Hence one can 'solve' (4.18) by iteration in terms of the initial conditions $\underline{s}_{(N)}$ and the fluctuation forces $\underline{f}_{(N)}(s) = N^{1/2}\underline{\varphi}_{(N)}(s)$. This iterative solution has coefficients which are uniformly bounded, and their $\bar{\omega}$-expectation values converge for $N \to \infty$. The computation of the Wightman functions starts from expressions of the type (3.42) in the manner given in Theorems 3.3 and 4.1.

QED

We conclude this section with some qualitative statements about the classical equations (4.7), which describe the approach to equilibrium of our class of systems to $O(N)$. We have already remarked that all solutions of (4.7) are global and uniformly bounded in t in terms of the initial conditions $\underline{\alpha}$. In the purely lossy case (i.e. $\eta^m = 0$ for $1 \leqslant m \leqslant M$, $\sigma^{ik}(\underline{\alpha}, t) \to 0$ for $t \to \infty$ and all $\underline{\alpha}$. For small pumping, η, the stationary solution (for certain β)

$$\sigma^{ij} = 0, \quad i \neq j,$$

$$\sigma^{kk} = \eta^k / 2\gamma^{kk} \tag{4.19}$$

persists as a stable attractor until it becomes unstable. For some critical value of the coefficients of (4.7) (e.g. of the pump parameters η^k, which are sometimes under the control of the experimenters), another attracting critical point or a closed orbit [H8] or even more complicated attractors [J1], [R4] can bifurcate from (4.19).

In many cases the set of attractors $A(\eta)$ will be piecewise analytic in η. At every η_c, where the structure of the attractors changes, we speak of a *reservoir-induced phase transition of an open system* which is in general far away from thermal equilibrium. Experimentally and theoretically, the best understood example is the laser threshold (see Section 5), but other phenomena in solid state physics, in chemistry [G1] and in biology [P1] might have a similar idealized microscopic explanation.

It is to be remembered that, for small pumping, every classical state converges to the pure classical state (4.19) as $t \to \infty$. Consequently the probability measure μ_ω^t loses its classical entropy.

If the system is in a normal classical state, then the linearized equations around the classical observables can have stability, asymptotic stability, or instability with respect to fluctuations. All three cases can occur: For instance the stable but not asymptotically stable case holds for attracting periodic solutions, e.g. for the laser above threshold. In that case, there is one characteristic exponent zero, and the fluctuations are not all damped in directions parallel to the periodic orbit. The fluctuation forces succeed, in a sense, to restore the broken symmetry in this case. It is tempting to identify the unstable attractors with metastable phases [W2]. In normal classical states, Onsager's hypothesis [O1] about the 'regression of fluctuations' is valid: The equations of motion for the fluctuations, when averaged over ω_R, are equal to the linearized equations of the intensive observables. This conjectured profound connection between transport theory and fluctuation theory can easily be derived in our mean field type models.

We have always taken the limit $N \to \infty$ first and then the limit $t \to \infty$. Physically one wants to take the limit the other way around. We can show in our models that such an interchange is justified if the damping is very large with respect to the coupling constants of the non-linearities in H^S. We do not expect this to hold for all values of the parameters, at least not at critical points. This accounts for the difference between our results and those of Risken [R1] and of Hempstead and Lax [H2] at the laser threshold.

5. Examples of Reservoir-Induced Phase Transitions

The mean field Josephson oscillator

As a first illustration we shall study a model of two strongly coupled superconductors. Let $\underline{k}_1, \ldots \underline{k}_N$ be the momenta characteristic of 1-electron states in the neighbourhood of the Fermi surface of a many electron system in a box of volume V. N and V are assumed to be proportional. The 1-electron states are denoted by

$$+n = (\underline{k}_n, \uparrow), \quad -n = (-\underline{k}_n, \downarrow), \tag{5.1}$$

where the arrow gives the spin state. Now imagine two such boxes, V, of electrons, and let $a^{\#}_{\pm n}$ and $b^{\#}_{\pm n}$ be their electron creation and annihilation operators with the usual anticommutation relations. Let us introduce quasi-spin operators for the two electron systems:

$$\begin{aligned} R^+_n &= a^*_n a_{-n} = (R^-_n)^*, \quad R^3_n = (a^*_n a_n - a^*_{-n} a_{-n})/2 \\ S^+_n &= b^*_n b_{-n} = (S^-_n)^*, \quad S^3_n = (b^*_n b_n - b^*_{-n} b_{-n})/2 \\ R^i_{(N)} &= \sum_{n=1}^{N} R^i_n, \quad S^i_{(N)} = \sum_{n=1}^{N} S^i_n. \end{aligned} \tag{5.2}$$

They are the generators of $\mathrm{Lie}(SU(2) \times SU(2)) = \mathscr{L}$. The total Hamiltonian of the system is

$$H^S_{(N)} = \epsilon(R^3_{(N)} + S^3_{(N)}) + \mu N^{-1}(R^+_{(N)} R^-_{(N)} + S^+_{(N)} S^-_{(N)}) + \lambda N^{-1}(R^+_{(N)} S^-_{(N)} + S^+_{(N)} R^-_{(N)}). \tag{5.3}$$

The first two terms are the usual BCS strong coupling Hamiltonians for the two boxes [T2], which we henceforth refer to as superconductors. The last term constitutes a tunnelling Hamiltonian which one might think of as a mean field Josephson junction.

The closed system shows a second-order phase transition [H5]. As a caricature of a driven Josephson junction from a constant current source, we shall assume that electrons have the R-superconductor by linear electron dissipation into a large empty normal electron reservoir and enter the S-superconductor from a full reservoir. The reservoir fermion field operators are denoted by $A^{\#}_{\pm nw}$ and $B^{\#}_{\pm nw}$ with $w \in \mathbf{R}$ and the usual anticommutation relations. According to Section 3, we consider states $\omega = \omega_S \otimes \omega_R$, where $\omega_R = (\Omega_R, \cdot \Omega_R)$, which satisfy

$$A_{\pm nw}\Omega_R = 0 = B^*_{\pm nw}\Omega_R \tag{5.4}$$

for all $\pm n$ and all w.

The linear dissipation is described by

$$H^R_{(N)} = \sum_{\pm n} H^R_{\pm n},$$

$$H^R_{\pm n} = \int dw (A^*_{\pm nw} A_{\pm nw} + B^*_{\pm nw} B_{\pm nw})\, w + \int dw (g^* A^*_{\pm nw} a_{\pm n} + g^* B^*_{\pm nw} b_{\pm n} + \mathrm{h.c.}), \tag{5.5}$$

where $\gamma = 2\pi|g|^2 > 0$.

The results of Section 4 apply to this model. We shall discuss the behaviour of the

intensive observables $\underline{\rho}_{(N)} = N^{-1}\underline{R}_{(N)}$ and $\underline{\sigma}_{(N)} = N^{-1}\underline{S}_{(N)}$ in classical states ω_S. The classical equations of motion are

$$\begin{aligned}
\dot{\rho}^+ &= (i\epsilon - \gamma)\rho^+ - 2i\mu\rho^+\rho^3 - 2i\lambda\sigma^+\rho^3,\\
\dot{\rho}^3 &= -\gamma(\rho^3 + \tfrac{1}{2}) + i\lambda(\rho^-\sigma^+ - \rho^+\sigma^-),\\
\dot{\sigma}^+ &= (i\epsilon - \gamma)\sigma^+ - 2i\mu\sigma^+\sigma^3 - 2i\lambda\rho^+\sigma^3,\\
\dot{\sigma}^3 &= -\gamma(\sigma^3 - \tfrac{1}{2}) + i\lambda(\sigma^-\rho^+ - \sigma^+\rho^-).
\end{aligned} \tag{5.6}$$

We remark that the dissipation does not couple operators from $\mathscr{L}$ to other operators in Lie $U(4)$. From (5.7) we obtain the time dependence of the Casimir functions $\underline{\rho}^2 = |\rho^+|^2 + (\rho^3)^2$ and $\underline{\sigma}^2$:

$$\begin{aligned}
\frac{d}{dt}\underline{\rho}^2 &= -2\gamma(|\rho^+|^2 + (\rho^3 + \tfrac{1}{4})^2 - \tfrac{1}{16}),\\
\frac{d}{dt}\underline{\sigma}^2 &= -2\gamma(|\sigma^+|^2 + (\sigma^3 - \tfrac{1}{4})^2 - \tfrac{1}{16}).
\end{aligned} \tag{5.7}$$

The physical region

$$D = \{|\underline{\rho}| \leqslant \tfrac{1}{2},\ |\underline{\sigma}| \leqslant \tfrac{1}{2}\} \tag{5.8}$$

is invariant under time evolution, and even if one starts outside of D, one would eventually come into D, as $t \to \infty$.

For the simplest typical case, let us set $\mu = 0$. Then the global flow can be discussed further, if one uses the following consequences of (5.6):

$$\frac{d}{dt}(\rho^3 + \sigma^3) = -\gamma(\rho^3 + \sigma^3), \tag{5.9}$$

$$\frac{d}{dt}(\rho^+ + i\sigma^+) = (i\epsilon - \gamma + 2\lambda\sigma^3)(\rho^+ + i\sigma^+) - 2i\lambda\sigma^+(\rho^3 + \sigma^3), \tag{5.10}$$

$$\frac{d}{dt}(\rho^+ - i\sigma^+) = (i\epsilon - \gamma - 2\lambda\sigma^3)(\rho^+ - i\sigma^+) - 2i\lambda\sigma^+(\rho^3 + \sigma^3). \tag{5.11}$$

One sees from (5.9) that $\rho^3(t) + \sigma^3(t) = (\rho^3(0) + \sigma^3(0))\exp -\gamma t$. For $\lambda < \gamma$ one deduces from (5.10) and (5.11), using $\sigma^3 \leqslant \frac{1}{2}$ for $(\underline{\rho}, \underline{\sigma}) \in D$, that both $\rho^+ + i\sigma^+$ and $\rho^+ - i\sigma^+$ converge to zero as $t \to \infty$. By going back to (5.6) one proves that the stationary solution

$$\begin{aligned}
&\rho^+ = \sigma^+ = 0,\\
&\rho^3 = -\sigma^3 = -\tfrac{1}{2}
\end{aligned} \tag{5.12}$$

is a global attractor for $\lambda < \gamma$.

For $\lambda \geqslant \gamma$, (5.12) becomes unstable, as the discussion of the linearized equations around (5.12) shows. If one writes (5.6) as a real system, then a pair of complex conjugate eigenvalues for the linearized system passes the imaginary axis from the left, away from the origin. By the Hopf bifurcation theorem [H8], a stable attracting periodic solution should bifurcate from (5.12). The harmonic Ansatz $\rho^+(t) = \rho^+ \exp i\omega t$, $\sigma^+(t) = \sigma^+ \exp i\omega t$ with time-independent ρ^+, σ^+, ρ^3, σ^3 and ω leads to the Hopf solution

$$\omega = \epsilon, \quad \sigma^3 = -\rho^3 = \gamma/2\lambda,$$

$$\rho^+ = i\sigma^+, \quad |\sigma^+|^2 = \gamma(1-\gamma/\lambda)/4\lambda. \tag{5.13}$$

Of course, the common phase of ρ^+ and σ^+ is not uniquely determined by (5.13), because of time translation invariance.

We see that this system of strongly coupled superconductors interacting with reservoirs of different 'voltages' can exist in two regimes: For $\lambda \leqslant \gamma$, the friction dominates, and $\underline{\rho}$ is drained and $\underline{\sigma}$ drowned by the reservoirs. For λ slightly larger than γ, the system becomes self-oscillatory. The asymptotic state of the system does not depend on the initial conditions (except on a set of codimension two and except for a phase factor). The mean field Josephson oscillator produces a periodic process at the expense of a non-periodic source of energy, just as a clock or a steam engine does.

The Dicke–Haken–Lax laser model

This model has already been physically characterized in the introduction. We take $H^S_{(N)}$ as in (1.1) and H^P as in (1.2) with $k(w) = k > 0$ and $\kappa = \pi k^2$ and $E(w) = w$. In this paper we want to avoid difficulties associated with unbounded boson operators. Therefore we shall consider a 'solid state laser', where the dissipation (or pumping) proceeds not by the coupling of two-level atoms with a reservoir consisting of two-level atoms but by an exchange of electrons with an electron reservoir.

The atomic 'spin' operators are represented, as in the Josephson model, in terms of two Fermi operators per atom n

$$S^+_n = b^*_n b_{-n} = (S^-_n)^*, \quad S^3_n = (b^*_n b_n - b^*_{-n} b_{-n})/2. \tag{5.14}$$

Each $b^\#_{\pm n}$ is coupled to its own Fermi bath with creation and annihilation operators $B^\#_{\pm nw}$ and $C^\#_{\pm nw}$ by

$$H^A_{(N)} = \sum_{\pm n} H^A_{\pm n}$$

$$H^A_{\pm n} = \int dw (B^*_{\pm nw} B_{\pm nw} + C^*_{\pm nw} C_{\pm nw})\, w + \int dw \{(f^*_\pm B^*_{\pm nw} + g^*_\pm C^*_{\pm nw})\, b_{\pm n} + \text{h.c.}\}. \tag{5.15}$$

The state Ω_R of the reservoir is again characterized by

$$A_w \Omega_R = B_{\pm nw} \Omega_R = C^*_{\pm nw} \Omega_R = 0, \tag{5.16}$$

and we assume customary commutation and anticommutation relations.

We choose the coupling constants in (5.15) to satisfy

$$|f_+|^2 + |g_+|^2 = |f_-|^2 + |g_-|^2,$$
$$|g_+|^2 = |f_-|^2, \tag{5.17}$$

which insures that the mean electron number per atom

$$\nu_{(N)} = N^{-1} \sum_{n=1}^{N} (b^*_n b_n + b^*_{-n} b_{-n}) \tag{5.18}$$

does not couple in $O(1)$ through the dissipation to the other operators $\underline{\sigma}_{(N)}$ and $\alpha_{(N)}$,

and has the stationary value 1 (macroscopic charge neutrality). There remain two free parameters describing the dissipation:

$$\gamma = 2\pi(|g_+|^2 + |g_-|^2),$$

$$\eta = (|g_+|^2 - |g_-|^2)/2(|g_+|^2 + |g_-|^2). \tag{5.19}$$

Then the macroscopic equations of the laser take the form (1.14), (1.15) and (1.16), except that in (1.16) the factor 2γ is changed into γ. This will neither change the laser frequency (5.39) nor the threshold condition (5.37), but only the slope of $|\alpha|^2_{\text{stat}}$ as a function of $\eta - \eta_c$ (5.40). It is not surprising that different models for the reservoirs can lead to different physical predictions in $O(N)$. The 'quantum mechanical consistency' [H1] allows for one more free parameter ($\delta > 0$ instead of 2γ in (1.16)) in the Dicke laser model.

The time dependence of the Casimir function becomes

$$\frac{d}{dt}\underline{\sigma}^2 = -2\gamma(|\sigma^+|^2 + (\sigma^3 - \eta/2)^2 - \eta^2/4), \tag{5.20}$$

and for $\mu = 0$ one has, in addition,

$$\frac{d}{dt}(|\alpha|^2 + \sigma^3) = -2\kappa|\alpha|^2 - \gamma(\sigma^3 - \eta). \tag{5.21}$$

One can prove [H6] and expects from the equilibrium thermodynamics of the system [H4] that the mean photon number per atom, $|\alpha|^2$, should approach a stationary value $|\alpha|^2_{\text{stat}} < \infty$ for every reasonable initial condition. In order to avoid having to deal with unbounded boson operators, we therefore introduce a high photon number cut-off at $a^* a = N\zeta$, where $\zeta \gg |\alpha|^2_{\text{stat}}$ is an arbitrarily large integer. Technically, we replace (see e.g. [A1])

$$a \to (\zeta N)^{-1/2} R^-_{(\zeta N)}. \tag{5.22}$$

Here the $R^i_{(\zeta N)}$ are spin operators in the irreducible representation of $SU(2)$ with spin $\zeta N/2$. If one replaces the n-photon states Ω_n by eigenstates Ω'_n of $R^3_{(\zeta N)}$ with eigenvalue $n - \zeta N/2$, then one has

$$\Omega'_n = (n!)^{-1}\binom{\zeta N}{n}^{-1/2}(R^+_{(\zeta N)})^n \Omega'_0, \tag{5.23}$$

$$R^+_{(\zeta N)}\Omega'_n(\zeta N)^{-1/2} = (n+1)^{1/2}\Omega'_{n+1}(1 - n/\zeta N)^{1/2},$$

$$[R^-_{(\zeta N)}, R^+_{(\zeta N)}]\Omega'_n(\zeta N)^{-1} = \Omega'_n(1 - 2n/\zeta N).$$

In the sense of (5.23), the $R^{\pm}_{(\zeta N)}(\zeta N)^{-1/2}$ act as photon creation and annihilation operators uniformly in N for mean photon numbers $n/N \ll \zeta$.

The final form of our Dicke Hamiltonian is

$$H^S_{(N)} = \nu(R^3_{(\zeta N)} + \zeta N/2) + \epsilon S^3_{(N)} + \zeta^{-1/2} N^{-1}(\lambda R^+_{(\zeta N)} S^-_{(N)} + \mu R^+_{(\zeta N)} S^+_{(N)} + \text{h.c.}). \tag{5.24}$$

There exists a model of a photon reservoir, which leads to the same phenomenological

dissipative part as (1.2) (up to $O(\zeta^{-1})$): One only has to introduce $2\zeta N$ Fermi operators $a^{\#}_{\pm m}$, $1 \leqslant m \leqslant \zeta N$ and

$$R^{+}_{m} = a^{*}_{m} a^{*}_{-m}, \quad R^{3}_{m} = (a^{*}_{m} a_{m} - a_{-m}\, a^{*}_{-m})/2,$$

$$R^{i}_{(\zeta N)} = \sum_{m=1}^{\zeta N} R^{i}_{n}, \tag{5.25}$$

$$a_{\pm m} \Omega_0' = 0, \quad 1 \leqslant m \leqslant \zeta N.$$

Then one couples the $a^{\#}_{\pm m}$ to Fermi reservoirs $A^{\#}_{\pm mw}$ by $H^{P}_{(N)} = \sum H^{P}_{\pm m}$, where

$$H^{P}_{\pm m} = \int dw \left(w A^{*}_{\pm mw} A_{\pm mw} + \frac{k}{\sqrt{2}} (A^{*}_{\pm mw} a_{\pm m} + \text{h.c.}) \right) \tag{5.26}$$

and $A_{\pm mw} \Omega_R = 0$.

For ζ fixed, the results of Section 4 apply for the intensive observables

$$\sigma^{i}_{(N)} = N^{-1} S^{i}_{(N)}, \quad \rho^{i}_{(\zeta N)} = (\zeta N)^{-1} R^{i}_{(\zeta N)}. \tag{5.27}$$

More useful for the limit $\zeta \to \infty$ will be

$$\alpha_{(\zeta, N)} = \zeta^{1/2} \rho^{-}_{(\zeta N)}. \tag{5.28}$$

The resulting equations of motion are

$$\dot{\alpha}_{(\zeta N)} = -(i\nu + \kappa)\, \alpha_{(\zeta, N)} + 2i\lambda \rho^{3}_{(\zeta N)} \sigma^{-}_{(N)} + 2i\mu \rho^{3}_{(\zeta N)} \sigma^{+}_{(N)} + \varphi_{(\zeta, N)}, \tag{5.29}$$

$$\dot{\sigma}^{-}_{(N)} = -(i\epsilon + \gamma)\, \sigma^{-}_{(N)} + 2i\lambda\, \sigma^{3}_{(N)} \alpha_{(\zeta, N)} + 2i\mu \sigma^{3}_{(N)} \alpha^{*}_{(\zeta, N)} + \chi^{+}_{(\zeta, N)}, \tag{5.30}$$

$$\dot{\sigma}^{3}_{(N)} = -\gamma(\sigma^{3}_{(N)} - \eta) + (i\lambda \sigma^{-}_{(N)} \alpha^{*}_{(\zeta, N)} + i\mu \sigma^{-}_{(N)} \alpha_{(\zeta, N)} + \text{h.c.}) + \chi^{3}_{(\zeta, N)}. \tag{5.31}$$

These equations are the same as in Section 1, except for different fluctuation forces and for the fact that there is $\rho^{3}_{(\zeta N)}$ instead of $\frac{1}{2}$ in (5.29). $\rho^{3}_{(\zeta N)}$ is not a c-number but satisfies

$$\dot{\rho}^{3}_{(\zeta N)} = -\kappa(\rho^{3}_{(\zeta N)} + \tfrac{1}{2}) + \varphi^{3}_{(\zeta, N)} + \zeta^{-1}(i\lambda \sigma^{+}_{(N)} \alpha_{(\zeta, N)} + i\mu \sigma^{+}_{(N)} \alpha^{*}_{(\zeta, N)} + \text{h.c.}). \tag{5.32}$$

We note, however, that if ζ is so large that the last term, which is $O(\zeta^{-1})$, can be neglected then, provided we start at time zero with $\rho^{3}_{(\zeta N)} = -\frac{1}{2}$, (5.29) reduces to (1.14).

We shall consider states $\omega = \omega_S \otimes \omega_R$ with ω_S classical with respect to $\underline{\rho}_{(\zeta N)}$ and $\underline{\sigma}_{(N)}$. Then the ω-expectation values of monomials in $\underline{\sigma}_{(N)}(t)$ and $\alpha_{(\zeta, N)}(t)$ can be expressed, in the limit *first* $N \to \infty$ *then* $\zeta \to \infty$ by the solutions of the classical equations

$$\begin{aligned} \dot{\alpha} &= -(i\nu + \kappa)\, \alpha - i\lambda \sigma^{-} - i\mu \sigma^{+}, \\ \dot{\sigma}^{-} &= -(i\epsilon + \gamma)\, \sigma^{-} + 2i\lambda \sigma^{3}\ \alpha + 2i\mu \sigma^{3}\, \alpha^{*}, \\ \dot{\sigma}^{3} &= -\gamma(\sigma^{3} - \eta) + (i\lambda \sigma^{-}\, \alpha^{*} + i\mu \sigma^{-}\, \alpha + \text{h.c.}), \end{aligned} \tag{5.33}$$

where the parameters satisfy

$$\gamma, \kappa, \epsilon, \nu > 0, \quad \lambda, \mu \in \mathbf{R}, \quad \lambda \neq 0. \tag{5.34}$$

For all μ there exists one time-independent stationary solution of (5.33):

$$\sigma^{3} = \eta, \quad \sigma^{-} = \alpha = 0. \tag{5.35}$$

For $\mu = 0$ (and hence for small $|\mu|$) this stationary solution is unique, since for $(\sigma^-, \alpha) \neq (0,0)$ the coefficient determinant of the equation $\dot{\sigma}^- = \dot{\alpha} = 0$ has to vanish. The latter is analytic in μ and, for $\mu = 0$, it takes the value $(i\nu + \kappa)(i\epsilon + \gamma) - 2\lambda^2\sigma^3 \neq 0$.

For the stability of (5.35) one has to discuss the linearized equations around (5.35):

$$\dot{\alpha} = -(i\nu + \kappa)\,\alpha - i\lambda\sigma^- - i\mu\sigma^+,$$

$$\dot{\sigma}^- = -(i\epsilon + \gamma)\,\sigma^+ + 2i\lambda\eta\alpha + 2i\mu\eta\alpha^*,$$

$$\dot{\sigma}^3 = -\gamma\sigma^3. \tag{5.36}$$

For $\mu = 0$, one root of the characteristic polynomial

$$z^2 + \{\kappa + \gamma + i(\nu + \epsilon)\}\,z - 2\lambda\eta + (i\nu + \kappa)(i\epsilon + \gamma) = 0$$

crosses the imaginary axis away from the origin, if

$$\eta = \frac{\kappa\gamma}{2\lambda^2}\left(1 + \frac{(\epsilon - \nu)^2}{(\kappa + \gamma)^2}\right) \equiv \eta_c, \tag{5.37}$$

Hence, for strong damping or far away from resonance (i.e. for $\eta_c > \frac{1}{2}$) the non-radiating solution is stable for all physical values of the pump parameter, namely $|\eta| \leqslant \frac{1}{2}$.

By the Hopf bifurcation theorem, a stable periodic solution will branch from (5.35), if $\eta > \eta_c$. This picture will persist for small μ, with small changes in η_c.

For $\mu = 0$ and $\eta_c < \eta$ there exists a one-parameter family of harmonic solutions of (5.33) of the type $\alpha(t) = \alpha \exp -i\omega t$, $\sigma^-(t) = \sigma^- \exp -i\omega t$ with time-independent α, σ^-, σ^3 and ω given by

$$\sigma^3 = \eta_c, \quad \sigma^- = (i\kappa + \omega - \gamma)\,\alpha/\lambda, \tag{5.38}$$

$$\omega = (\nu\gamma + \epsilon\kappa)(\gamma + \kappa)^{-1}, \tag{5.39}$$

$$|\alpha|^2 = \gamma(\eta - \eta_c)/2\kappa. \tag{5.40}$$

This solution lies in the physical region $|\sigma| \leqslant \frac{1}{2}$. Note that σ^3 is independent of the pump parameter η and that the mean photon number increases linearly with η above threshold. These formulae are well-known from semi-classical laser theory [H1] and are in fair agreement with experiments on finite lasers [D2]. In the gas laser, $\gamma/2\kappa$ has to be replaced by γ/κ in (5.40).

This harmonic solution is stable near threshold. We have verified stability for all $\eta - \eta^c$, if either $2\kappa = \gamma$ or $\nu = \epsilon$. In the former case one can even show, that (5.38, 5.39, 5.40) is the unique stable attractor of the system: (5.36) with $\mu = 0$ is equivalent to (5.21) and

$$\ddot{\beta} + [i(\epsilon + \nu - 2\omega) + \kappa + \gamma]\,\dot{\beta} + 2\lambda^2(\eta_c - \sigma^3)\,\beta = 0, \tag{5.41}$$

where

$$\beta(t) \equiv \alpha(t) \exp - i\omega t.$$

For

$$2\kappa = \gamma, \quad \sigma^3(t) \to \eta - |\beta(t)|^2$$

exponentially. Hence the attractors can be determined from (5.41) with σ^3 replaced by $\eta - |\beta|^2$. This equation has a Ljapounov function

$$H(\beta, \dot{\beta}) = |\dot{\beta}|^2 + \lambda^2|\beta|^4 + 2\lambda^2(\eta_c - \eta)|\beta|^2 \tag{5.42}$$

with $\dot{H} = -6\kappa|\dot{\beta}|^2$, and $\dot{H} = 0$ only for $\dot{\beta} = 0$. Hence for every integral curve $\dot{\beta}(t) \to 0$, which entails $\sigma^3(t) \to \eta_c$ and hence $|\beta(t)|^2 \to \eta - \eta_c$.

We see that the laser, too, shows a non-equilibrium phase transition at η_c (provided that $\eta_c < \frac{1}{2}$) between a unique non-radiating time-independent macrostate and a 1-parameter family of stable 'self-oscillatory' attracting macrostates. In both regimes, the fluctuation theory can be worked out and we hope to return to this interesting question in the future.

Conclusion

The main point of this paper is to exhibit a many-body system showing irreversible behaviour, where one can really separate classical and quantum effects. It has always been the faith of physicists that, for reservoirs which are very large with respect to the system of interest, the effect of the reservoir can be described to $O(N)$ by phenomenological classical dissipative equations and by a Langevin-type linear fluctuation theory in $O(\sqrt{N})$ around the classical macrostate. We have solved a non-linear quantum mechanical model (without using uncontrolled approximations such as master equations, quasilinearization and 'adiabatic' elimination procedures), where the conventional wisdom of irreversible statistical mechanics far from thermal equilibrium can be deduced from a microscopic theory.

It incidentally happens to be the case that our theory leads to a model of the laser and that it gives qualitative predictions which have some resemblance to experimental facts.

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Equilibrium Statistical Mechanics of Matter Interacting with the Quantized Radiation Field

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The thermodynamic properties of several systems of multilevel atoms interacting with a quantized radiation field are investigated. We allow a quantum-mechanical treatment of the translational degrees of freedom and do not require the rotating-wave approximation. In the finite-photon-mode case one can calculate the free energy per atom in the thermodynamic limit exactly and rigorously. In the infinite-mode case we only get upper and lower bounds, but these are sufficient to give conditions for thermodynamic stability and instability. The kind of phase transition previously found by us for the one-mode Dicke model with the rotating-wave approximation persists in the general multimode case.

I. INTRODUCTION

In a previous paper[1] we elucidated the thermodynamic properties of the Dicke maser model with one photon mode coupled to N two-level atoms in the rotating-wave approximation. We calculated the free energy per atom and the thermal expectation values of time-dependent intensive and fluctuation observables exactly in the limit $N \to \infty$. Our analysis relied heavily on the various conservation laws inherent in the model: the total "number" operator and the total atomic "spin." In the relevant part of the spectrum we effectively diagonalized the Hamiltonian in such a way that the error became negligible as $N \to \infty$. While such a procedure is necessary if one wants to study fluctuation observables, it is intuitively clear that a simpler mean field method must exist if one is content to analyze only the intensive observables. In fact our results showed that these quantities behave classically; that is to say the lack of commutativity becomes unimportant as $N \to \infty$. It is also clear that these qualitative features should continue to hold even without the above mentioned conservation laws, i.e., it should be possible to handle a much wider class of models. In this paper we show how to achieve that goal in a simple way by using coherent states and the results of a recent paper.[2] The phase transition found in Ref. 1 persists in the general multimode case.

Wang and Hioe[3] and Hioe[4] demonstrated that the Glauber coherent states of the photon field constitute a natural basis for this problem. Unfortunately, they were not able to show that their approximate evaluation of $N^{-1} \ln \mathrm{Tr} e^{-\beta H}$ is exact when $N \to \infty$. Nevertheless, it is a fact that their answer agreed precisely with our previous rigorous result[1] for the Dicke model, and we shall prove here that their results for the other models they treat are also correct. In addition, we also calculate exactly the expectation values of intensive observables for those models. Ginibre[5] has previously made use of coherent states to obtain exact results for the many-boson problem. Our methods can be easily generalized for atoms of more than two levels.

In Sec. III we make an attempt to understand the thermodynamics of the infinite-mode case which, to the best of our knowledge, was never discussed before. We cannot solve that problem exactly, but we can derive upper and lower bounds to the partition function which prove that such a system is thermodynamically stable if and only if the atoms have very repulsive cores.

In Sec. IV we return to the finite-mode Hamiltonian, but allow translational degrees of freedom (either quantum or classical) for the atoms. It is shown there that use of the Glauber coherent photon states permits an exact (as $N \to \infty$) reduction of the problem to a conventional many body problem. This, in turn, can be solved in closed form in several interesting cases.

We do not confine our attention only to the Glauber coherent photon states, but also show that the Bloch atomic coherent states[6] for the atoms may be used to advantage. The former make the radiation field classical, while the latter make the atomic variables classical. It is the Bloch states that are used in our discussion of the infinite-mode case.

In the Appendix we resolve some technical problems related to the unbounded nature of the photon operators.

II. FINITE-MODE MODELS

The Hamiltonians we shall consider are those of the form

$$H=\sum_{m=1}^{M}\nu_m a_m^* a_m+\epsilon S^z$$
$$+N^{-1/2}\sum_{m=1}^{M}\sum_{n=1}^{N}[a_m(\lambda_{mn}S_n^+ +\mu_{mn}S_n^-)+\text{H.c.}], \quad (2.1)$$

where $a_1^\#,\ldots,a_M^\#$ are boson creation and annihilation operators for the photon modes having energies $\nu_m>0$, $\vec{S}_1,\ldots,\vec{S}_N$ are spin-$\frac{1}{2}$ operators describing N two-level atoms having energy spacing $\epsilon>0$ ($S_n^+=S_n^x+iS_n^y$ and $S^i=\sum_{n=1}^N S_n^i$, $i=x,y$ or z). The λ_{mn} (respectively, μ_{mn}) are coupling constants for the rotating (respectively, counter-rotating) wave terms. The factor $N^{-1/2}$ in (2.1) really comes from a factor $V^{-1/2}$, where V is the volume of the cavity containing the atoms. However, as we are interested in N/V fixed, the distinction merely entails a coupling constant renormalization. The interaction term in (2.1) is linear in the $a^\#$ operators, but the method we are about to describe would work equally well if one included quadratic terms (i.e., if one goes beyond the dipolar approximation).

A. Atomic Coherent State Representation

We turn now to the atomic or Bloch angular momentum coherent states[6] used in Ref. 2. With $\mathfrak{F}$ being the Fock space for all the photon modes and $\mathfrak{K}$ being the Hilbert space for the N atoms (spins) we define

$$Z=\text{Tr}e^{-\beta H} \quad (2.2)$$

where the trace is over $\mathfrak{F}\otimes\mathfrak{K}$. The bounds obtained in Ref. 2, and justified in the Appendix for boson operators, are

$$\tilde{Z}(\tfrac{1}{2})\le Z\le\tilde{Z}(\tfrac{3}{2}), \quad (2.3)$$

where

$$\tilde{Z}(J)=2^N\,\text{Tr}_{\mathfrak{F}}(4\pi)^{-N}\int d\Omega^N e^{-\beta\tilde{H}(J,\Omega^N)} \quad (2.4)$$

and where

$$\Omega^N=(\vec{\Omega}_1,\ldots,\vec{\Omega}_N),$$
$$\vec{\Omega}_n=(\sin\theta_n\cos\varphi_n,\sin\theta_n\sin\varphi_n,\cos\theta_n). \quad (2.5)$$

$\tilde{H}(J,\Omega^N)$ is defined from (2.1) by replacing each $\vec{S}_n$ by $J\vec{\Omega}_n$. The bounds in (2.3) for the free energy per atom do not agree as $N\to\infty$, but they are useful in proving the stability of the infinite photon mode free energy—a subject to which we shall return in Sec. III.

Further progress can be made with the Bloch-state bounds, however, if we make an assumption about H, namely that the λ_{mn} and the μ_{mn} are independent of n. This is true in the original Dicke model where one neglects the spatial variation of the radiation field. (Alternatively, the method will work if the atoms belong to a finite number of groups in each of which the coupling constants are the same.) In this case we can use the fact that the total "spin," J, is a constant of the motion, so that

$$Z=\sum_{J\ge 0}^{N/2}Y(N,J)Z(J), \quad (2.6)$$

$$Z(J)=\text{Tr}e^{-\beta H(J)}, \quad (2.7)$$

where $H(J)$ is the Hamiltonian for a spin, $\vec{S}$, of magnitude J,

$$H(J)=\sum_{m=1}^{M}\nu_m a_m^* a_m+\epsilon S^z$$
$$+N^{-1/2}\sum_{m=1}^{M}[a_m(\lambda_m S^+ +\mu_m S^-)+\text{H.c.}] \quad (2.8)$$

and

$$Y(N,J)=N!\,(2J+1)[(J+1+\tfrac{1}{2}N)!\,(\tfrac{1}{2}N-J)!]^{-1} \quad (2.9)$$

is the number of ways to construct an angular momentum J from N spin-$\frac{1}{2}$ particles.

Using Ref. 2, one has the bounds

$$\tilde{Z}(J)\le(2J+1)^{-1}Z(J)\le\tilde{Z}(J+1), \quad (2.10)$$

with

$$\tilde{Z}(J)=(4\pi)^{-1}\,\text{Tr}_{\mathfrak{F}}\int d\Omega e^{-\beta\tilde{H}(J,\Omega)} \quad (2.11)$$

and $\tilde{H}(J,\Omega)$ is (2.8) with S replaced by $J\vec{\Omega}$. Since $\tilde{H}$ is quadratic in the $a_m^\#$, it is easy to evaluate $\text{Tr}_{\mathfrak{F}}$ in (2.11):

$$\tilde{Z}(J)=(4\pi)^{-1}\prod_{m=1}^{M}(1-e^{-\beta\nu_m})^{-1}\int_0^\pi\sin\theta\,d\theta\int_0^{2\pi}d\varphi\,\exp\left(-\beta\epsilon J\cos\theta+\beta N^{-1}J^2\sin^2\theta\sum_{m=1}^{M}|\lambda_m e^{i\varphi}+\mu_m e^{-i\varphi}|^2\nu_m^{-1}\right). \quad (2.12)$$

Since $J^2\le\frac{1}{4}N^2$, we see that

$$\ln\tilde{Z}(J+1)-\ln\tilde{Z}(J)\le\beta\epsilon+\beta[(N+1)/N]\sum_{m=1}^{M}(|\lambda_m|+|\mu_m|)^2\nu_m^{-1}, \quad (2.13)$$

which means that (2.12) gives the free energy per atom exactly to order M/N. It is also clear that for large N and fixed M, (2.12) and (2.6) can be evaluated by steepest descent, i.e., simply by maximizing with respect to θ, φ, and J. If we first maximize with respect to φ we see that *the free energy is the same as that for one mode in the rotating-wave approximation,* but with an effective coupling constant λ given by

$$\lambda^2 = \max_\varphi \sum_{m=1}^{M} |\lambda_m e^{i\varphi} + \mu_m e^{-i\varphi}|^2 \nu_m^{-1}. \tag{2.14}$$

Subsequent maximization with respect to θ and J yields the free energy found in Ref. 1. Such a result agrees with that found in Ref. 3.

Expectation values of intensive observables can be found by the foregoing procedure, but some technicalities are required. These will be discussed in the Appendix. The result is as expected: The expectation value of any polynomial in the intensive observables (defined in the Appendix) is equal to that polynomial evaluated at the maximal steepest descent points referred to above, and then averaged over the variety of maximal steepest descent points if there is more than one point.

Before turning to the photon coherent states, which we shall describe next, we remark that when there is no spatial dependence (λ_{mn} and μ_{mn} independent of n) the Bloch picture (2.12) is the more convenient to use. The main conclusion, (2.14), that even without the rotating-wave approximation there is effectively only one coupling constant, is more tedious to derive using the photon coherent states (cf. Refs. 3 and 4).

B. Photon Coherent-State Representation

For a given photon mode, a^*, a Glauber coherent state is

$$|\alpha\rangle = \exp[-\tfrac{1}{2}|\alpha|^2 + \alpha a^*]|0\rangle, \tag{2.15}$$

where α is any complex number and $|0\rangle$ is the photon vacuum. The following properties are required and are justified in the Appendix:

$$\langle\alpha|\beta\rangle = \exp[-\tfrac{1}{2}|\alpha|^2 - \tfrac{1}{2}|\beta|^2 + \alpha^*\beta], \tag{2.16}$$

$$\mathrm{Tr}|\alpha\rangle\langle\beta| = \langle\beta|\alpha\rangle, \tag{2.17}$$

$$\mathrm{Tr}A = \pi^{-1}\int d\alpha \langle\alpha|A|\alpha\rangle, \tag{2.18}$$

where A is any trace-class operator and $\int d\alpha = \iint_{-\infty}^{\infty} d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha)$,

$$\langle\alpha|a|\alpha\rangle = \alpha, \tag{2.19}$$

$$\langle\alpha|a^*a|\alpha\rangle = |\alpha|^2, \tag{2.20}$$

$$I = \pi^{-1}\int d\alpha |\alpha\rangle\langle\alpha|, \tag{2.21}$$

$$a = \pi^{-1}\int d\alpha\alpha |\alpha\rangle\langle\alpha|, \tag{2.22}$$

$$a^*a = \pi^{-1}\int d\alpha(|\alpha|^2 - 1)|\alpha\rangle\langle\alpha|. \tag{2.23}$$

The same methods as in Ref. 2, but using the Glauber states instead of the Bloch states, yield upper and lower bounds for the partition function (again, see the Appendix):

$$\bar{Z} \le Z \le \exp\left(\beta \sum_{m=1}^{M} \nu_m\right)\bar{Z}, \tag{2.24}$$

where

$$\bar{Z} = \pi^{-M}\,\mathrm{Tr}_{\mathcal{H}}\int d\alpha^M e^{-\beta\tilde{H}(\alpha^M)}, \tag{2.25}$$

and

$$\alpha^M = (\alpha_1, \ldots, \alpha_M),$$

$$\tilde{H}(\alpha^M) = \sum_{m=1}^{M} \nu_m|\alpha_m|^2 + \epsilon S^z + N^{-1/2} \times \sum_{m=1}^{M}\sum_{n=1}^{N}[\alpha_m(\lambda_{mn}S_n^+ + \mu_{mn}S_n^-) + \mathrm{H.c.}]. \tag{2.26}$$

The trace on $\mathcal{H}$ in (2.25) is now easy to compute:

$$\bar{Z} = \pi^{-M}\int d\alpha^M \exp\left(-\beta\sum_{m=1}^{M}\nu_m|\alpha_m|^2\right) 2^N \prod_{n=1}^{N} \cosh \times \left[\tfrac{1}{2}\beta\left(\epsilon^2 + 4N^{-1}\left|\sum_{m=1}^{M}(\alpha_m\lambda_{mn} + \alpha_m^*\mu_{mn})\right|^2\right)^{1/2}\right]. \tag{2.27}$$

This $\bar{Z}$ is precisely the approximate partition function derived by Wang and Hioe.[3,4] We note from (2.24) that, as long as the number of photon modes is finite, $-\beta N^{-1}\ln\bar{Z}$ is the free energy per atom to order MN^{-1}. Another remark is that although we assumed each atom to have only two levels, the atomic trace in (2.26) can just as well be evaluated for multilevel atoms, and the interaction does not have to be linear in the atomic $S^\pm$ operators.

III. THERMODYNAMIC STABILITY OF THE INFINITE-MODE SYSTEM

In this section we return to the Hamiltonian H of (2.1) and shall show that under suitable conditions it is stable when the number of photon modes is infinite. This means that there exists a constant A such that $Z = \mathrm{Tr}e^{-\beta H} < e^{NA}$ for all N. The proof of the existence of the thermodynamic limit, $\lim_{N\to\infty} N^{-1}\ln Z$, is a more complicated question with which we shall not deal. The phrase infinite number of modes means that in any frequency interval (ν_1, ν_2) the number of modes with $\nu_1 < \nu < \nu_2$

is proportional to N, the size of the cavity. The problem we are considering here is similar to the corresponding problem for electron-phonon interactions dealt with by Gallavotti, Ginibre, and Velo.[7]

We use the bounds (2.3) and the definition (2.4). The trace over the photon modes $\mathfrak{F}$ can easily be done exactly and one finds, dropping irrelevant factors of the form $e^{\text{const}\,N}$,

$$\tilde{Z}(J) \sim R_N \int d\Omega^N \exp\left(\beta J^2 \sum_{n=1}^{N}\sum_{j=1}^{N} v(\vec{\Omega}_n, \vec{\Omega}_j) - \beta\epsilon J \sum_{n=1}^{N} \cos\theta_n\right), \tag{3.1}$$

where

$$v(\vec{\Omega}_n, \vec{\Omega}_j) = N^{-1} \sum_m \nu_m^{-1} \mathrm{Re}(\lambda_{mn} S_n^+ + \mu_{mn} S_n^-) \times (\lambda_{mj}^* S_j^- + \mu_{mj}^* S_j^+), \tag{3.2}$$

$$S_n^{\pm} = \sin\theta_n e^{\pm i\varphi_n}, \tag{3.3}$$

and R_N is the ideal photon contribution to Z

$$R_N = \prod_m (1 - e^{-\beta\nu_m})^{-1}. \tag{3.4}$$

The latter is independent of the interaction and may be assumed to have a nice thermodynamic limit in a physically sensible model, e.g.,

$$\nu_m \to \nu(\vec{k}) = |\vec{k}|, \tag{3.5}$$

$\vec{k} = 2\pi N^{-1}(n_x, n_y, n_z), n_i \in Z, \vec{k} \neq 0$. We could allow several photon modes for each $\vec{k}$; such a generalization does not affect the conclusions below.

If (3.2) be inserted into (3.1), one has (dropping R_N) precisely the partition function of N classical spins of magnitude J interacting with each other via a quadratic interaction and with an external magnetic field ϵ in the z direction. This is a well understood problem. If one allows all the particles to be at the same location, i.e., λ_{mn} and μ_{mn} independent of n, then $v(\vec{\Omega}_n, \vec{\Omega}_j)$ is positive when $\vec{\Omega}_n \approx \vec{\Omega}_j$, and no matter what one assumes about the various parameters, the *lower* bound $\tilde{Z}(\frac{1}{2})$ will behave like e^{BN^2} with $B > 0$. Thus, *no stability is possible in this case* and, as we shall show later, the introduction of the quantum mechanical uncertainty principle does not save the situation.

To describe (3.2) more concretely, we use (3.5) *et seq.*; we associate a position $\vec{x}_n$ with each atomic index n, and suppose that

$$\lambda_{mn} \to \lambda(\vec{k}) e^{i\vec{k}\cdot\vec{x}_n}, \qquad \mu_{mn} \to \mu(\vec{k}) e^{i\vec{k}\cdot\vec{x}_n}. \tag{3.6}$$

Then

$$v(\vec{\Omega}_n, \vec{\Omega}_j) \to \sum_{i=1}^{4} g^i(\vec{\Omega}_n, \vec{\Omega}_j) h^i(\vec{x}_n - \vec{x}_j), \tag{3.7}$$

where

$$h^1(\vec{x}) = N^{-1} \sum_{\vec{k}} \nu(\vec{k})^{-1} [|\lambda(\vec{k})|^2 + |\mu(\vec{k})|^2] \cos(\vec{k}\cdot\vec{x}), \tag{3.8}$$

$$g^1(\vec{\Omega}_n, \vec{\Omega}_j) = \sin\theta_n \sin\theta_j e^{i(\varphi_n - \varphi_j)}, \tag{3.9}$$

and the other pairs $g^i, h^i, r = 2, 3, 4$ are defined similarly.

Let us investigate how the generic $h(\vec{x})$ decreases as $|\vec{x}| \to \infty$. In a real system, $\lambda(\vec{k})$ and $\mu(\vec{k})$ are the Fourier transforms of functions with exponential decrease at infinity, i.e.,

$$\lambda(\vec{k}) = \int d^3x \psi_u^*(\vec{x}) \vec{e}(\vec{k}) \cdot \vec{p} \psi_l(\vec{x}) e^{i\vec{k}\cdot\vec{x}}, \tag{3.10}$$

where u and l refer to the upper and lower atomic states, $\vec{e}$ is a polarization vector and $\vec{p}$ is the momentum operator. Since $\lambda(\vec{0}) \neq 0$, there is an infrared problem connected with the potential (3.8). On physical grounds we do not think this difficulty is intractable but, as a somewhat painful analysis is required, we shall not try to solve this problem here. For one thing, one should certainly include the term $\vec{A}^2$ in the Hamiltonian, where $\vec{A}$ is the vector potential. This introduces a positive quadratic form in the a^* operators which can be handled by our methods, just as the photon energy, $\sum \nu_m a_m^* a_m$, was. It will certainly mitigate the k^{-1} divergence in (3.8).

From now on we shall assume $\lambda(\vec{k})$ has a zero of sufficiently high order at $\vec{k} = 0$. Then

$$h^i(\vec{x}) = \sum_{n \in Z^3} \bar{h}(\vec{x} + \vec{n}L), \tag{3.11}$$

where L is the length of the cubic cavity and $\bar{h}(\vec{x})$ is a smooth, real function which decreases at infinity as $|\vec{x}|^{-4}$, for example. For such a potential, it is well known[8] that the total N body potential appearing in (3.1) is stable provided the particles are not too close together, e.g., $|\vec{x}_i - \vec{x}_j| > a > 0$ for all i, j.

To generalize the above model, (2.1), we can permit the atomic coordinates $\{\vec{x}_n\}$ to be variable and replace H by $H + U(\vec{x}_1, \ldots, \vec{x}_N)$, where U is some ordinary interatomic potential, e.g., a sum of pair potentials. Now the partition function involves a configurational integral on $(R^3)^N$, i.e.

$$Z \to (N!)^{-1} \int_{V^N} d^{3N}x \, Z(x) e^{-\beta U(x)}, \tag{3.12}$$

where $Z(x)$ is the partition function for each fixed set of atomic positions as defined in (2.2). The bounds (2.3) still apply and we can draw the following general conclusion: If we ignore the infrared problem as above, then the total Ham-

iltonian is stable if U is sufficiently repulsive whenever two atoms get close together and if U decays sufficiently fast (i.e., faster than $|x|^{-3-\epsilon}$ for $\epsilon>0$) at large separations. Conversely, the Hamiltonian is unstable if U does not have strongly repulsive cores.

The next level of complication is to treat the atomic coordinates quantum-mechanically, i.e., $H \to H+U+T$, where T is the N-particle kinetic energy operator. Using Bloch states we can still derive the bounds (2.3), but now

$$\tilde{Z}(J) = 2^N \operatorname{Tr}_{\mathfrak{F}} \operatorname{Tr}_{\mathfrak{G}} \int d\Omega^N \exp[-\beta \tilde{H}(J, \Omega^N) + U(x) + T], \tag{3.13}$$

where $\mathfrak{G}$ is the Hilbert space $L^2(V^N)$ and $\tilde{H}$ is as in (2.4). Because the terms linear in $a^\#$ involve the x_n's, it is no longer possible to do the trace over $\mathfrak{F}$ in a closed form. To circumvent this difficulty, we derive upper and lower bounds to (3.13).

Lower bound. We use the variational principle $\operatorname{Tr} e^A > e^{(\psi, A\psi)}$ for any normalized ψ. With Ω^N fixed we choose $\psi \in \mathfrak{F} \otimes \mathfrak{G}$ to be $\psi = \varphi \otimes \rho$. Let ρ be of the form $\rho(\vec{x}_1, \ldots, \vec{x}_N) = \prod_{n=1}^{N} \rho_i(\vec{x}_i)$ where the ρ_i are smooth functions with supports in V which are pair-wise disjoint. Since the supports are disjoint we can imagine the atoms to be either fermions or bosons without affecting any expectation values. With ρ given, we can calculate $(\psi, T\psi)$ and $(\psi, V\psi)$. Recalling that λ_{mn} depends upon $\vec{x}_n$, we can calculate $\langle \lambda_{mn} \rangle = (\psi, \lambda_{mn}\psi)$, and similarly $\langle \mu_{mn} \rangle$. Now we choose $\varphi \in \mathfrak{F}$ to be the ground-state eigenvector of

$$\sum \nu_m a_m^* a_m + N^{-1/2} \sum \sum \{a_m \langle \lambda_{mn} \rangle S_n^+ + \langle \mu_{mn} \rangle S_n^- + \text{H.c.}\} \tag{3.14}$$

with energy

$$-N^{-1} \sum_m \nu_m^{-1} \left| \sum_n \langle \lambda_{mn} \rangle S_n^+ + \langle \mu_{mn} \rangle S_n^- \right|^2 . \tag{3.15}$$

The point of this lower bound calculation is to show that the quantum uncertainty principle does not change the previous conclusion based on classical mechanics, namely that a repulsive core is still needed in U. Without it we still have that $Z > e^{CN^2}$ for large N with $C > 0$; this can be accomplished by letting all ρ_i have support in some fixed box of size l, where l is such that the ground-state energy of (3.14) is still $O(N^2)$ and negative. Then, $(\psi, T\psi) = O(N^{5/3} l^{-2})$, and hence the ground-state energy of $H+T$ is still $O(N^2)$ and negative.

Upper bound. We can write the Hamiltonian $H+T+U$ as $H_1 + H_2$, where $H_1 = T + \frac{1}{2}\sum \nu_m a_m^* a_m$ and $H_2 = H' + U$, and where H' is as in (2.1), except that it has a factor $\frac{1}{2}$ multiplying the photon-energy term. The kinetic energy does not appear in H_2, and if U has the aforementioned repulsive core plus rapid fall-off properties then the factor $\frac{1}{2}$ in H' does not affect the previous conclusion: as an operator on $\mathfrak{F} \otimes \mathfrak{G}$, H_2 is bounded below by $-BN$ for some constant B. Thus

$$Z < e^{\beta B N} \operatorname{Tr}_{\mathfrak{F}} \operatorname{Tr}_{\mathfrak{G}} e^{-\beta H_1} < e^{AN}$$

for some constant A.

In summary, a proper quantum statistical treatment of the atomic center of mass motion does not affect the general conclusion above.

IV. FINITE-MODE CASE WITH TRANSLATIONAL DEGREES OF FREEDOM

In Sec. III we were obliged to use the Bloch atomic state picture for a simple, but fundamental reason: If one uses the Glauber state picture, one sees from (2.20) and (2.23) that the difference between the upper and lower bounds to the free energy (2.24) is precisely $\sum_{m=1}^{M} \nu_m$, and if the number of modes is infinite this sum generally diverges. On the other hand, if M is finite one can always use the Glauber state picture, and the difference of the bounds is $O(N^{-1})$ in the free energy per atom. With this in mind, we shall briefly consider the class of Hamiltonians mentioned at the end of Sec. III, but with M finite, i.e.,

$$K = H + U + T, \tag{4.1}$$

where K is the total Hamiltonian in the Hilbert space $\mathfrak{K} = \mathfrak{F} \otimes \mathfrak{G} \otimes \mathfrak{K}$, H is given by (2.1), U is an ordinary interatomic potential and T is the N-atom kinetic energy.

Our bounds lead to the statement that to $O(1)$ in the total free energy

$$Z \equiv \operatorname{Tr}_{\mathfrak{K}} e^{-\beta K}, \tag{4.2}$$

$$Z = \pi^{-M} \int d\alpha^M Z(\alpha), \tag{4.3}$$

and

$$Z(\alpha) = \operatorname{Tr}_{\mathfrak{K} \otimes \mathfrak{G}} e^{-\beta K(\alpha)}, \tag{4.4}$$

where $K(\alpha)$ is K with a_m and a_m^* replaced by the c numbers α_m and α_m^*. By changing variables $\alpha_m \to \gamma_m N^{1/2}$, it is clear that one can use steepest descent (in the limit $N \to \infty$) to evaluate the integral (4.3). With $\gamma = (\gamma_1, \ldots, \gamma_M)$, we define

$$g(\gamma) = \lim_{N \to \infty} N^{-1} \ln Z(N^{1/2}\gamma). \tag{4.5}$$

Then,

$$\lim_{N \to \infty} N^{-1} \ln Z = \max_\gamma g(\gamma), \tag{4.6}$$

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provided the set on which the maximum occurs is of dimension less than $2M$. The existence of the limit $g(\gamma)$ can be shown by customary methods[8] when U is reasonable. It is generally impossible to calculate $g(\gamma)$ exactly, but the point is that the problem has been reduced to a conventional problem of point particles with spin interacting via a spin independent potential U and whose spins are coupled to a static external field which may or may not have a spatial variation. If U is a sum of single particle potentials, $g(\gamma)$ can be evaluated in closed form and there will clearly be a phase transition for sufficiently large coupling constants λ_{mn}, μ_{mn} from $\gamma = 0$ to $\gamma \neq 0$ as β is varied, just as there is in the models considered in Sec. II. An example of this in which the translational degrees of freedom are treated classically is given in Ref. 4. If U is more complicated, this kind of phase transition in γ probably still persists.

V. CONCLUSION

In this paper we have attempted to show the usefulness of coherent states (both Glauber states for the photon field and Bloch atomic states for the atomic degrees of freedom) to calculate rigorously the free energy per atom for various models of the interaction of matter and radiation. For the finite mode case (Sec. II) the problem can be reduced to the calculation of a classical type integral which can be handled by steepest descent methods. This proves the results of Hioe and Wang, and the Glauber state picture shows that, in effect, each atom interacts with a classical radiation field whose value is determined self-consistently. Therefore, one sees that as long as the number of photon modes is held fixed and as long as the interactions of the photons and atoms has a smooth spatial dependence, the thermodynamic properties of the model are very insensitive to the details of the Hamiltonian. In particular they are insensitive to whether or not the rotating-wave approximation is used and they are insensitive to the number of atomic levels, provided that number is finite.

The Bloch picture shows clearly that for two-level atoms with or without the rotating-wave approximation, but with spatially independent coupling constants, the problem reduces to that of a single photon mode in the rotating wave approximation. Furthermore, as shown in the Appendix, expectation values of intensive observables can be calculated using the mean fields given by the steepest-descent points of the coherent-state integrals. In this context we note a similarity to those approximations in laser theory in which the photon field is treated semiclassically, and in which the atoms are treated as independent, but fully quantum-mechanical entities.[9,10]

Section III explores the question of stability of the more fundamental Hamiltonian in which there are an infinite number of photon modes. Leaving aside the infrared problem, we have established some necessary and some sufficient conditions for the thermodynamic stability. Our methods are not powerful enough, however, to prove the existence of the thermodynamic limit.

In Sec. IV, where Hamiltonians similar to those of Sec. III but with a finite number of photon modes are discussed, the existence of the thermodynamic limit can be established. The main result of Sec. IV is that the inclusion of translational degrees of freedom generally does not destroy the kind of phase transition possessed by the models of Sec. II.

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APPENDIX: SOME TECHNICAL CONSIDERATIONS AND CALCULATION OF EXPECTATION VALUES

To avoid unnecessary complications we shall consider a one-mode Hamiltonian

$$H = H_0 + R,$$
$$H_0 = a^* a, \tag{A1}$$
$$R = A + a^* B + aB^*,$$

where the Hilbert space is $\mathcal{K} = \mathcal{F} \otimes \mathcal{H}$, $\mathcal{F}$ is the Fock space of the boson mode a^*, $\mathcal{H}$ is a finite dimensional Hilbert space of dimension d (the spin space) and A and B are operators on $\mathcal{H}$ with A Hermitian.

Clearly R is a Kato perturbation[11] of H_0, which implies that H is self-adjoint on $D(H_0)$, the domain of H_0; H is bounded from below and has purely discrete spectrum with finite multiplicity because H_0 has these properties. Therefore $\rho = e^{-\beta H_0}$ is bounded. To prove that ρ is trace class, write $\rho = \exp[-\frac{1}{2}\beta H_0 - \beta(\frac{1}{2}H_0 + R)]$. By the Golden-Thompson inequality,[12]

$$\mathrm{Tr}\rho \leq \mathrm{Tr} e^{-\beta H_0/2} e^{-\beta(H_0/2+R)}. \tag{A2}$$

The first factor in (A2) is trace class and the second is bounded.

Let P_n be the projector onto the states with $\leq n$ photons, so that $P_n \to I$ strongly. Let $H_n = P_n H P_n$ and consider

$$Z_n \equiv \mathrm{Tr} P_n e^{-\beta H_n}, \tag{A3}$$

which is a finite dimensional trace. We note that $D = \bigcup_n P_n \mathcal{K}$ is a common core for all H_n and H and,

for any $\psi \in D$, $P_n H P_n \psi = \psi$ for n sufficiently large. In fact $P_n Q P_n \psi = \psi$ for n sufficiently large when Q is any polynomial in a, with coefficients which are operators on $\mathcal{K}$. Hence $H_n \to H$ in the strong resolvent sense.[13] Let $\{\psi_i, h_i\}_{i=1}^{\infty}$ (resp. $\{\psi_i^n, h_i^n\}_{i=1}^{nd}$) be the eigenvectors and eigenvalues of H (resp. $H_n | P_n \mathcal{K}$) arranged in increasing order. We can use the ψ_i^n as trial vectors for H and conclude from the mini-max principle that $h_i^n \geq h_i$ for $1 \leq i \leq nd$. Using this fact, together with the strong convergence[13] of the eigenprojections $E_n(a,b) \to E(a,b)$ for every interval (a,b) with $a, b \notin \text{spec}(H)$, one can show that $h_i^n \to h^i$ and $\psi_n^i \to \psi^i$ weakly. Hence $Z_n \to Z$ by the dominated-convergence theorem.

Define the cutoff Glauber states by

$$|\alpha, n\rangle = P_n |\alpha\rangle . \tag{A4}$$

For these states the formulas (2.16)–(2.23) are correct with certain obvious modifications, i.e.,

$$\langle \alpha, n | \beta, n\rangle = K_n(\alpha, \beta) = \exp[-\tfrac{1}{2}|\alpha|^2 - \tfrac{1}{2}|\beta|^2] \times \sum_{m=0}^{n} (\alpha^* \beta)^m / m! , \tag{A5}$$

$$\mathrm{Tr} |\alpha, n\rangle\langle \beta, n| = K_n(\beta, \alpha) , \tag{A6}$$

$$\mathrm{Tr} P_n A P_n = \pi^{-1} \int d\alpha \langle \alpha, n | A | \alpha, n\rangle , \tag{A7}$$

$$\langle \alpha, n | a | \alpha, n\rangle = \alpha K_{n-1}(\alpha, \alpha) , \tag{A8}$$

$$\langle \alpha, n | a^* a | \alpha, n\rangle = |\alpha|^2 K_{n-1}(\alpha, \alpha) , \tag{A9}$$

$$P_n = \pi^{-1} \int d\alpha |\alpha, n\rangle\langle \alpha, n| , \tag{A10}$$

$$P_n a P_n = \pi^{-1} \int d\alpha \alpha |\alpha, n\rangle\langle \alpha, n| , \tag{A11}$$

$$P_n a^* a P_n = \pi^{-1} \int d\alpha (|\alpha|^2 - 1) |\alpha, n\rangle\langle \alpha, n| , \tag{A12}$$

$$\pi^{-1} \int d\alpha K_n(\beta, \alpha) K_n(\alpha, \gamma) = K_n(\beta, \gamma) . \tag{A13}$$

Similar formulas hold for all other polynomials in $a^\#$.

We wish to compute a lower bound to Z_n following Ref. 2. Use (A7) and the fact that $\langle \psi | e^X | \psi \rangle \geq \langle \psi | \psi \rangle \exp(\langle \psi | X | \psi \rangle / \langle \psi | \psi \rangle)$ applied to H_n. Then

$$Z_n \geq \mathrm{Tr}_{\mathcal{K}} \int d\alpha K_n(\alpha, \alpha) \times \exp\{-|\alpha|^2 K_{n-1}(\alpha, \alpha)/K_n(\alpha, \alpha) + A + [B\alpha^* K_{n-1}(\alpha, \alpha)/K_n(\alpha, \alpha) + \text{H.c.}]\} . \tag{A14}$$

First we take $\mathrm{Tr}_{\mathcal{K}}$, and then let $n \to \infty$. By the dominated-convergence theorem, the left side of (2.24) is proved. It is equally clear that the same strategy proves the lower bounds (2.3) and (2.4) obtained from the Bloch state representation.

It is somewhat more difficult to prove the upper bounds (2.24) or (2.3). According to the method of Ref. 2 one defines

$$Z_n^m = \mathrm{Tr} P_n (1 - \beta H_n / m)^m \tag{A15}$$

and, since the trace is finite dimensional, $\lim_{n\to\infty} Z_n^m = Z_n$. The difficulty is that if one applies (A5)–(A13) directly to (A15) the dominated convergence theorem will not be clearly valid. Instead, for all $\epsilon \geq 0$ we define $H_n(\epsilon)$ as follows. For each photon operator that appears in H_n, such as $a^* a$ or $a^\#$, one introduces a convergence factor $e^{(-\epsilon|\alpha|^2)}$ in the integrands of (A11) and (A12). Using $H_n(\epsilon)$, one defines $Z_n(\epsilon)$ and $Z_n^m(\epsilon)$. Then $\lim_{\epsilon \downarrow 0} Z_n(\epsilon) = Z_n$ and $\lim_{m\to\infty} Z_n^m(\epsilon) = Z_n(\epsilon)$. Using the Golden-Thompson inequality, as shown in Ref. 2, one has

$$Z_n^m(\epsilon) \leq \pi^{-1} \int d\alpha K_n(\alpha, \alpha) \mathrm{Tr}_{\mathcal{K}} \{1 - \beta \hat{H}(\alpha, \epsilon)\}^m , \tag{A16}$$

where $\hat{H}(\alpha, \epsilon)$ is defined by the replacements $a^* a \to (|\alpha|^2 - 1) e^{(-\epsilon|\alpha|^2)}$, etc. Owing to the convergence factor and to the Gaussian decrease of $K_n(\alpha, \alpha)$ [cf. (A5)] one can use dominated convergence to assert that

$$Z_n(\epsilon) \leq \pi^{-1} \int d\alpha K_n(\alpha, \alpha) \mathrm{Tr}_{\mathcal{K}} e^{\{-\beta \hat{H}(\alpha, \epsilon)\}} . \tag{A17}$$

Again, we can let $\epsilon \downarrow 0$ and use dominated convergence to replace $Z_n(\epsilon)$ by Z_n and $\hat{H}(\alpha, \epsilon)$ by $\hat{H}(\alpha, 0)$ in (A19). Now, because $\hat{H}$ has a term $|\alpha|^2$, we can let $n \to \infty$ and use dominated convergence to obtain the right-hand side of (2.24). For the Bloch state upper bound, (2.3), the same strategy works except that it is not necessary to introduce the convergence factor, i.e., one can deal directly with Z_n.

Having proved that the bounds on the partition function used in the main text can be justified for the unbounded photon operators, we turn now to the problem of evaluating expectation values of intensive observables. This latter is the algebra generated by $a^\#/N^{1/2}$ and by the atomic operators $S_{(N)}^i/N$. In particular we consider an operator Θ which is a monomial in the $a^\#/N^{1/2}$ times an operator on $\mathcal{K}$. Defining

$$\langle \Theta \rangle = \mathrm{Tr} \Theta e^{-\beta H} / \mathrm{Tr} e^{-\beta H} , \tag{A18}$$

we want to show that as $N \to \infty$, $\langle \Theta \rangle$ can be evaluated by simply replacing each factor in Θ by its value at the absolute maximum of the integrands of (2.11), (2.25), etc., and then *summing over those points*. [Note that in the Dicke model with the rotating-wave approximation there is a conservation law which leads to a gauge invariance. The

stationary phase "points" are, in fact, curves. After integrating over those curves, one finds, for example, that $N^{-1}\langle a^*a\rangle \neq 0$ but $N^{-1}\langle a^2\rangle = 0$, as expected (cf. Ref. 1)].

We shall need two lemmas whose use will become clear later. First we give a different proof and a slightly generalized version of Griffiths's lemma.[14]

Lemma 1 (Griffiths). Let $\{g_n(x)\}$ be a sequence of convex functions on $x \in (a,b) \equiv I \subset \mathbf{R}$ with a pointwise limit $g(x)$, which, of course, is convex. Let $G_n^+(x)$[resp. $G_n^-(x)$] be the right (resp. left) derivatives of $g_n(x)$, and similarly for $G^+(x)$, $G^-(x)$. Then, for all $x \in I$,

$$\limsup_{n\to\infty} G_n^+(x) \leq G^+(x)\,, \qquad \liminf_{n\to\infty} G_n^-(x) \geq G^-(x)\,. \tag{A19}$$

In particular, if all the $g_n(x)$ and $g(x)$ are differentiable at some point $x \in I$, then

$$\lim_{n\to\infty} dg_n(x)/dx = dg(x)/dx\,. \tag{A20}$$

Proof. Fix $x \in I$. For $y > 0$ and $x \pm y \in I$,

$$g_n(x+y) \geq g_n(x) + yG_n^+(x)\,,$$

$$g_n(x-y) \geq g_n(x) - yG_n^-(x)\,.$$

Fix y and take the limit $n \to \infty$. Then

$$\limsup_{n\to\infty} G_n^+(x) \leq y^{-1}[g(x+y) - g(y)]$$

and similarly for $\liminf_{n\to\infty} G_n^-(x)$. Now let $y \to 0$. Q.E.D.

In the following, Lemma 2, we consider a sequence of "partition functions" which, quite generally, we may write as

$$Z_n(\beta) = \int e^{-\beta n e} d\mu_n(e)\,, \tag{A21}$$

where $\{\mu_n\}$ is some sequence of nonnegative measure on $\mathbf{R}$. We assume that all $Z_n(\beta) < \infty$ for β in some open interval $I = (a,b)$. Define

$$g_n(\beta) = n^{-1} \ln Z_n(\beta)\,. \tag{A22}$$

Obviously, $g_n(\beta)$ is convex for $\beta \in I$. We also define the moments of the energy (per particle) as

$$E_n^k(\beta) = \int e^k e^{-\beta n e} d\mu_n(e)/Z_n(\beta)\,, \tag{A23}$$

where $k = 0, 1, 2, \ldots$. It is easy to prove (by dominated convergence, or otherwise) that for $\beta \in I$, $E_n^k(\beta)$ exists and

$$E_n^k(\beta) = (-n)^{-k} Z(\beta)^{-1} d^k Z_n(\beta)/d\beta^k. \tag{A24}$$

Lemma 2. Let the sequence $\{\mu_n, Z_n(\beta), g_n(\beta)\}$ be defined as above and assume that

$$\lim_{n\to\infty} g_n(\beta) = g(\beta) \tag{A25}$$

exists. Then, for every β at which $g(\beta)$ is differentiable,

$$\lim_{n\to\infty} E_n^k(\beta) = [\lim_{n\to\infty} E_n^1(\beta)]^k = [-dg(\beta)/d\beta]^k. \tag{A26}$$

Proof. For $k = 1$, the lemma is the same as Lemma 1. Let J be a compact subinterval of I. From the facts that $Z_n(\beta) < \infty$ for all $\beta \in I$, and the uniform convergence of $g_n(\beta)$ on compacts, which always holds for convex functions, we can say that if $\beta \in J$ then we can find a lower cutoff e_0 in the integral (A23) such that the error in $g_n(\beta)$ and in $E_n^k(\beta)$ is $O(e^{-cn})$ for all k less than some fixed K, and where $c > 0$ is a constant independent of n and β. By adding a (trivial) constant to e we may assume, without loss of generality, that $e_0 = 1$, i.e., $\mu((-\infty, 1)) = 0$. Then $E_n^k(\beta) > 0$ and $e^k d\mu_n(e)$ is a non-negative measure for all k. Consider $k = 2$. Replace $d\mu_n(e)$ by $e d\mu_n(e)$ and thereby define $Z_n^1(\beta)$ and $g_n^1(\beta)$ as in (A23) and (A24). Then $dg_n^1(\beta)/d(\beta) = -E_n^2(\beta)/E_n^1(\beta)$. Now $\exp[n(g_n^1(\beta) - g_n(\beta))] = Z_n^1(\beta)/Z_n(\beta)$, so $h_n(\beta) \equiv g_n^1(\beta) - g_n(\beta) \to 0$. Hence, $g_n^1(\beta) = h_n(\beta) + g_n(\beta)$ is a convex function having the limit $g(\beta)$, and we can apply Lemma 1 to it on int(J). This proves the $k = 2$ case. Obviously, the argument can be extended inductively, i.e., one writes $E_n^k(\beta) = \prod_{j=1}^k [E_n^{k-j+1}(\beta)/E_n^{k-j}(\beta)]$. Q.E.D.

Now we return to the monomial $\mathcal{O}$ whose expectation value we wish to compute. If $\mathcal{O}$ is not self-adjoint then consider $\mathcal{O}$ to be replaced by $\mathcal{O} + \mathcal{O}^*$. Clearly there is some integer $k \geq 1$ such that H^k dominates $\mathcal{O}$, i.e., $|\mathcal{O}| \leq \frac{1}{2}H^k + bI$ for some positive constant b. With $\beta > 0$ fixed, let $e_k = \lim_{N\to\infty} N^{-k}\langle H^k\rangle$. For each $\lambda \geq 0$ define $H(\lambda) \equiv H + \lambda N\mathcal{O} + \lambda W$, with $W = N^{-k+1}H^k - e_{k-1}H$. Obviously, the preceding analysis for Z applies equally well to $Z(\lambda) \equiv \mathrm{Tr} e^{-\beta H(\lambda)}$, i.e., one can obtain upper and lower bounds to $Z(\lambda)$ in terms of classical integrals. Naturally, for the monomials in $\mathcal{O}$ and H^k one has to find the obvious generalizations of (2.19)–(2.23), but this can easily be done; in particular the monomial $(a^*)^p a^q$ has $(\alpha^*)^p \alpha^q$ as its leading term in (2.19)–(2.23).

The Peierls-Bogoliubov inequality

$$Z(\lambda) \geq Z(0) e^{-\beta\lambda\langle W\mathcal{O}+W\rangle}\,, \tag{A27}$$

can easily be proved to hold here. Then, with $g(\beta, N, \lambda) \equiv N^{-1} \ln Z(\lambda)$ and $\lambda > 0$,

$$\beta\langle\mathcal{O}\rangle \geq \lambda^{-1}[g(\beta, N, 0) - g(\beta, N, \lambda)] - \beta N^{-1}\langle W\rangle\,. \tag{A28}$$

Take the limit $N \to \infty$. In those cases (Secs. II and IV) in which our upper and lower bounds agree, they will also agree when $\lambda > 0$. Thus, $\lim_{N\to\infty} g(\beta, N, \lambda) = g(\beta, \lambda)$ exists. Also, $\lim_{N\to\infty} N^{-1}\langle W\rangle = 0$ by Lemma 2. Thus, for all $\lambda > 0$

$$\liminf_{N\to\infty}\langle\Theta\rangle \geq \lambda^{-1}[g(\beta,\lambda)-g(\beta,0)]. \tag{A29}$$

In a parallel way, we can define $H'(\lambda)=H-\lambda N\Theta+\lambda W$ and $g'(\beta,N,\lambda)$, and obtain

$$\limsup_{N\to\infty}\langle\Theta\rangle \leq \lambda^{-1}[g(\beta,0)-g'(\beta,\lambda)]. \tag{A30}$$

To complete the demonstration one has to show that as $\lambda \downarrow 0$ the right-hand sides of (A29) and (A30) have a common limit and that this is the classical value of $\langle\Theta\rangle$ at the steepest-descent points for $\lambda=0$. When these points are isolated, as they are in the absence of the rotating-wave approximation, it is easy to see that the above is true; as $\lambda \downarrow 0$ some points approach the $\lambda=0$ points while others go off to infinity. The latter are not maximal, however. In the rotating-wave approximation, the $\lambda=0$ points are in fact curves $|\alpha|=$const. In this case, (A29) and (A30) will agree for those operators such as a^*a/N or $aS^+/N^{3/2}$ which are invariant under the gauge group. For other operators, such as a^2, the two limits will not agree because as $\lambda \downarrow 0$ the steepest-descent curves will be approached as two different points. However, in such cases it is easy to see directly that $\langle a^2\rangle=0$, and this value agrees with what one would get if one integrated over the entire curve.

This completes our discussion of the Hamiltonian (A1) and clearly no difficulty is encountered in extending it to the multimode case. However, some remarks are needed for the Hamiltonians considered in Secs. III and IV because the unbounded operators T and/or U are introduced. The additional Hilbert space, $\mathcal{G}$, is generally $L^2(V^N)$, where V is the box, but if U has a hard core it is $L^2(V^N-\text{hard-core region})$. In either case, it suffices to say that in addition to the P_n photon projection operators one can also introduce a strongly convergent sequence of projections $\{Q_n\}$ on $\mathcal{G}$ such that $D=\cup_n Q_n\mathcal{G}$ is a common core for H and all Q_nHQ_n and such that $(Q_nHQ_n-H)\varphi\to 0$ strongly for all $\varphi\in D$.

The remarks in this appendix are admittedly sketchy in places, but the interested reader can easily fill in the details required to analyze any particular model of the class we have considered in the main text.

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With K. Hepp in Springer Lecture Notes in Physics *25*, 298–316 (1973)

CONSTRUCTIVE MACROSCOPIC QUANTUM ELECTRODYNAMICS

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§1. Introduction

After ten days of difficult lectures the audience and the lecturers need some holidays. I have chosen the subject of this last talk half for your recreation, half for exposing you to some new and exotic aspects of the quantum world of infinitely many degrees of freedom, where there are many interesting problems in mathematical physics. My lecture will be centered around the quantum electrodynamics of the laser in the thermodynamic limit, on which E.H.Lieb and I have worked for some time. It is hard to give fair references in this field with a continuous transition to applied physics. A good starting point on laser theory is the book by Haken [H1] as well as various contributions in [A1] , [G3] , [K1]. The statistical theory of instabilities in stationary nonequilibrium systems is treated in [G1] and [G4] with many references to older contributions. A general approach to nonequilibrium phase transitions in mean field models with linear dissipation has been given in [H4] , with great emphasis on the nonlinear analysis of the Heisenberg equations of motion. In this lecture I shall presenta simplified approach to these problems, using only linear functional analysis and working in the Schrödinger picture. By this method one can easily incorporate the unbounded boson operators of the quantized radiation field, and one sees better the analogy to the usual treatment of the classical limit in quantum mechanics [H5] , [M1] .

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§2. Heuristic Discussion of the Laser

The Dicke Haken Lax model of the 1-mode 2-level homogeneously broadened laser starts from the following approximation to the Hamiltonian of quantum electrodynamics

$$H = \sum_{m=1}^{\infty} \gamma_m a_m^* a_m + \varepsilon \sum_{n=1}^{N} S_n^3 + V^{-1/2} \sum_{m=1}^{\infty} \sum_{n=1}^{N} \{ a_m (\lambda_{mn} S_n^+ + \mu_{mn} S_n^-) + \text{h.c.} \} . \quad (2.1)$$

Here the $a_m^{\#}$ are creation and annihilation operators for the discrete set of photon modes of energy γ_m of a cavity of volume V. The λ_{mn} and μ_{mn} are coupling constants for the rotating and counter-rotating interaction of the mode m with the n^{th} atom. We assume finitely many atoms, N, in the cavity and shall later take $N = V$ in the passage to the thermodynamic limit. The atoms have two states with fermion creation and annihilation operators $b_{+n}^{\#}$ and $b_{-n}^{\#}$ for the upper and lower level and no translational degrees of freedom. Then

$$S_n^+ = b_{+n}^* b_{-n} = (S_n^-)^* \quad , \quad S_n^3 = (b_{+n}^* b_{+n} - b_{-n}^* b_{-n})/2 \quad (2.2)$$

satisfy SU_2 commutation relations

$$[S_n^3, S_n^{\pm}] = \pm S_n^{\pm} \quad , \quad [S_n^+, S_n^-] = 2S_n^3 \quad , \quad [S_n^i, S_m^j] = 0 \quad \text{for} \quad m \neq n \quad . \quad (2.3)$$

Little is known in general about the system described by (2.1), except for thermodynamic stability with hard cores and instability without a sufficiently strong repulsion at short distances [H3]. For finitely many modes, an equilibrium phase transition from a normally radiating to a superradiant phase can be established [H2].

In these lectures we are interested in the nonequilibrium behaviour of the system, and we shall restrict ourselves to one mode and, for notational convenience, to the rotating wave approximation :

$$H_N^S = \gamma a^* a + \varepsilon S_N^3 + \lambda N^{-1/2} (S_N^+ a + a^* S_N^-) , \quad (2.4)$$

where only the total spin operators enter :

$$S_N^i = \sum_{n=1}^{N} S_n^i \quad . \quad (2.5)$$

The total Hamiltonian H_N of the laser cavity with $N \sim V$ atoms and photons coupled to atomic pumping devices and photonic loss mechanisms is of the form $H_N = H_N^S + H_N^R$, where the reservoir part will be given later, (4.1), (4.6), once we have acquired a qualitative understanding of the laser action. Since the S_N^i give a representation of SU_2, it is natural to consider the Heisenberg equations of motion for the five operators $S_N^k(t) = \exp(iH_N t)\, S_N^k \exp(-iH_N t)$ and $a_N^{\#}(t)$:

$$\begin{aligned}
\dot{a}_N(t) &= -i\gamma a_N(t) - i\lambda N^{-1/2} S_N^-(t) + i\left[H_N^R, a_N(t)\right], \\
\dot{S}_N^-(t) &= -i\varepsilon S_N^-(t) + 2i\lambda N^{-1/2} S_N^3(t) a_N(t) + i\left[H_N^R, S_N^-(t)\right], \\
\dot{S}_N^3(t) &= i\lambda N^{-1/2}\left(a_N^*(t) S_N^-(t) - a_N(t) S_N^+(t) \right) + i\left[H_N^R, S_N^3(t)\right].
\end{aligned} \tag{2.6}$$

The very successful semiclassical theory of the laser [L1] suggests that H_N^R should be chosen in such a way that

$$\begin{aligned}
i\left[H_N^R, a_N(t)\right] &= -\varkappa a_N(t) + g_N(t), \\
i\left[H_N^R, S_N^-(t)\right] &= -\gamma S_N^-(t) + F_N^-(t), \\
i\left[H_N^R, S_N^3(t)\right] &= -\delta\left(S_N^3(t) - \eta N \right) + F_N^3(t).
\end{aligned} \tag{2.7}$$

Here $\varkappa > 0$ and $\gamma > 0$ are damping constants for the photon amplitude and the atomic polarisation, while $\delta > 0$ and $-1/2 \le \eta \le 1/2$ should describe the pumping of the atoms into a mean inversion $\eta \approx S_N^3/N$. Of course, the purely dissipative terms alone on the r.h.s. of (2.7) are inconsistent with the selfadjointness of H_N. However, one hopes that in a suitable topology the additional fluctuation forces $g_N(t)$ and $F_N^k(t)$ become negligible in the limit $N \to \infty$. Assume that $g_N(t) = O(1)$ and $F_N^k(t) = O(N^{1/2})$, by some law of large numbers. Then it is plausible that the intensive observables

$$\begin{aligned}
\alpha_N^{\#}(t) &= a_N^{\#}(t) N^{-1/2}, \\
\sigma_N^k(t) &= S_N^k(t) N^{-1},
\end{aligned} \tag{2.8}$$

which at $t = 0$ have $O(N^{-1})$ commutators, become c-numbers in the limit $N \to \infty$, and satisfy the ordinary differential equations

$$\dot{\alpha} = -(i\gamma + \varkappa)\alpha - i\lambda\sigma^- ,$$

$$\dot{\sigma}^- = -(i\varepsilon + \delta)\sigma^- + 2i\lambda\sigma^3\alpha , \tag{2.9}$$

$$\dot{\sigma}^3 = -\delta(\sigma^3 - \eta) + i\lambda(\sigma^-\alpha^* - \sigma^+\alpha) .$$

These equations have remarkable properties which correspond quite well to the qualitative picture of laser action. It can be rigorously shown [H4] that they have global solutions in (2.10) for all physical initial conditions

$$\begin{aligned} &\alpha \in \mathbb{C} , \qquad \sigma^- \in \mathbb{C} , \\ &\sigma^3 \in \mathbb{R} , \qquad (\sigma^3)^2 + |\sigma^-|^2 \leq 1/4 . \end{aligned} \tag{2.10}$$

There exists a unique stationary solution

$$\sigma^3 = \eta , \quad \alpha = \sigma^- = 0 , \tag{2.11}$$

and a 1-parameter family of periodic solutions, $\sigma^-(t) = \sigma^- \exp -i\omega t$, $\alpha(t) = \alpha \exp -i\omega t$, $\sigma^3(t) = \sigma^3$, if and only if $1/2 \geq \eta > \eta_c$, where

$$\eta_c = \frac{\varkappa\delta}{2\lambda^2}\left(1 + \frac{(\varepsilon-\gamma)^2}{(\varkappa+\delta)^2}\right) , \quad \sigma^3 = \eta_c ,$$

$$|\alpha|^2 = \delta(\eta-\eta_c)/2\varkappa , \quad \omega = \frac{\varkappa\varepsilon + \delta\gamma}{\varkappa+\delta} , \tag{2.12}$$

$$\lambda\sigma^- = (i\varkappa + \omega - \gamma)\alpha .$$

At $\eta = \eta_c$, a Hopf bifurcation [H6] occurs : below threshold the laser is damping dominated, and the mean photon number per atom, $|\alpha|^2$, goes to zero from any initial state, while above threshold the stationary value $|\alpha|^2 = \delta(\eta-\eta_c)/2\varkappa$ is attained for $t \to \infty$, starting from almost any initial condition. These equations suggest that a nonequilibrium phase transition occurs at laser threshold and that the attracting self-oscillatory state is one of the dissipative structures which have been discussed by Prigogine and coworkers [G1]. In the following we shall give a Hamiltonian model H_N^R and an asymptotic expansion in $N^{1/2}$ in which this heuristic picture holds rigorously in $O(N)$.

§3. The Classical Limit for Atoms and the Radiation Field

There are several topologies in which the infinite volume limit can be studied. A very concrete and rather elementary discussion is possible in the Schrödinger picture, by passing with $N \to \infty$ along a sequence of photon and atomic coherent states [G2] using the Trotter theory of approximating Hilbert spaces [T2]. These coherent states exhaust all physical initial conditions for the intensive observables, and hence they can be considered as the true pure classical states of the infinite system. However, if one measures finer properties of the system by looking at the fluctuation observables, then one finds [H2] that the physical stationary states are not coherent, but that they can be described in the Hilbert space generated from a coherent state by applying all polynomials in fluctuation operators. In this section we shall consider the classical limit for the closed system of atoms and radiation. The interaction H_N^S has the form (2.4), and we shall first construct initial states $|\alpha, \underline{\sigma}\rangle_N = \Omega_N$ which are coherent in $a^\#$ and S_N^k.

Let $\alpha \in \mathbb{C}$, $U(\alpha) = \exp(\alpha a^* - \alpha^* a)$ and $|0\rangle$ be the ground state of $a^* a$. Then the sequence of photon coherent states $|N^{1/2}\alpha\rangle = U(N^{1/2}\alpha)|0\rangle$ satisfies

$$\langle N^{1/2}\alpha | \Pi (a^\# - N^{1/2}\alpha^\#) | N^{1/2}\alpha \rangle = \langle 0 | \Pi a^\# | 0 \rangle , \tag{3.1}$$

$$\lim_{N\to\infty} \langle N^{1/2}\alpha | \Pi (a^\# N^{-1/2}) | \alpha N^{1/2} \rangle = \Pi \alpha^\# . \tag{3.2}$$

The analogue to (3.1) and (3.2) for fermions can be constructed using the representation theory of SU_2 [G2]. Any $\underline{\sigma} \in \mathbb{R}^3$ with $\|\underline{\sigma}\| = \sigma \leq 1/2$ has the form $\underline{\sigma} = R\,\underline{\sigma}_0$, where $R \in SO(3)$ and $\sigma_0^k = -\sigma\,\delta_{0,}^k$ $1 \leq k \leq 3$. For simplicity, we restrict σ to a dense set of physical initial conditions :

$$\sigma = q/(2q + 4p) , \quad 0 \leq p,q \in \mathbb{Z} , \quad q > 0 . \tag{3.3}$$

Take $A \in SU_2$ acting on the Pauli matrices as $A^* \tau^k A = \sum_{i=1}^{3} \tau^i R^{ik}$ and define new fermion annihilators by

$$(b_{+n}, b_{-n}) = (c_{+n}, c_{-n})\, A \tag{3.4}$$

Let $|\pm\rangle$ be the states for the fermion pair $b_\pm$, where

$$c^*_{-n}|-\rangle = c_{+n}|-\rangle = 0\ ,\quad T^+|-\rangle = |+\rangle\ , \tag{3.5}$$

where $T^+ = c^*_+ c_-$. Then in obvious notation

$$|\underline{\sigma}\rangle_N = 2^{-pM/2}\left[(|+\rangle|-\rangle - |-\rangle|+\rangle)^p \otimes (|-\rangle)^q\right]^{\otimes M}. \tag{3.6}$$

Here $N = M(2p+q)$ and $M = 1,2,\ldots$ Let $T^i_N = \sum R^{ki} S^k_N$. Then

$$T^3_N|\underline{\sigma}\rangle_N = -\sigma N|\underline{\sigma}\rangle_N\ ,\quad T^-_N|\underline{\sigma}\rangle_N = 0 \tag{3.7}$$

defines an irreducible representation of SU_2. The fluctuation operators

$$t^+_N = N^{-1/2}T^+_N = (t^-_N)^*\ ,\quad t^3_N = N^{-1/2}T^3_N + \sigma N^{1/2} \tag{3.8}$$

satisfy [W1]:

$$\lim_{N\to\infty} {}_N\langle\underline{\sigma}|t^k_N\ldots t^m_N|\underline{\sigma}\rangle_N = \begin{cases}(\Omega_\infty, t^k_\infty\ldots t^m_\infty\,\Omega_\infty)\ , & \text{if all } k,..m = \pm\\ 0\ , & \text{otherwise.}\end{cases} \tag{3.9}$$

where $t^-_\infty\Omega_\infty = 0$ and $[t^-_\infty, t^+_\infty] = 2\sigma$. Let $t^\pm_\infty = t^1_\infty \pm i t^2_\infty$ and $t^3_\infty = 0$ and $\underline{s}_\infty = R\,\underline{t}_\infty$. Then

$$\lim_{N\to\infty} {}_N\langle\underline{\sigma}|\Pi N^{1/2}(\sigma^{k(m)}_N - \sigma^{k(m)})|\underline{\sigma}\rangle_N = (\Omega_\infty, \Pi s^{k(m)}_\infty\,\Omega_\infty)\ , \tag{3.10}$$

$$\lim_{N\to\infty} {}_N\langle\underline{\sigma}|\Pi\sigma^{k(m)}_N|\underline{\sigma}\rangle_N = \Pi\,\sigma^{k(m)}. \tag{3.11}$$

Although all our results can be expressed in terms of correlation functions and their limits, the mathematics simplifies considerably by introducing a sequence of approximating Hilbert spaces $\mathcal{H}_N$ which converges against $\mathcal{H}_\infty$, the GNS Hilbert space for (3.1) and (3.10). Let $\Omega_N = |N^{1/2}\alpha\rangle \otimes |\underline{\sigma}\rangle_N$ and $\mathcal{H}_N$ be the span of all $(a^* - N^{1/2}\alpha^*)^r (t^+_N)^s \Omega_N$. Define $I_N : \mathcal{H}_\infty \to \mathcal{H}_N$ by linear extension of

$$I_N(a^*_\infty)^r (t^+_\infty)^s\,\Omega_\infty = (a^* - N^{1/2}\alpha^*)^r (t^+_N)^s \Omega_N\ . \tag{3.12}$$

Then $\|I_N\| = 1$, and $\lim_{N\to\infty}\|I_N\varphi_\infty\| = \|\varphi_\infty\|$ for all $\varphi_\infty \in \mathcal{H}_\infty$, by (3.9).

On the finite particle subspace, $\mathcal{H}^{0}_{\infty}$, one has

$$\lim_{N\to\infty} \| x_N \cdots y_N I_N \varphi_\infty - I_N x_\infty \cdots y_\infty \varphi_\infty \| = 0 \quad , \tag{3.13}$$

if $x_N, \ldots y_N \in \{ (a^{\#} - N^{1/2}\alpha^{\#}), N^{1/2}(\underline{\sigma}_N - \underline{\sigma}) \}$. In a somehow different sense than in [H4], the intensive observables $\alpha^{\#}_N$, $\underline{\sigma}_N$ have normal fluctuations around $\alpha^{\#}$, $\underline{\sigma}$ in the sequence Ω_N of coherent states [W1].

We shall say that a sequence of selfadjoint operators A_N on $\mathcal{H}_N$ converges in the Weyl-Trotter sense to a selfadjoint operator A_∞ on $\mathcal{H}_\infty$, $A_N \xrightarrow{WT} A$, if for all $s \in \mathbb{R}$ and all $\varphi_\infty \in \mathcal{H}_\infty$

$$\lim_{N\to\infty} \| \exp(iA_N s)\, I_N \varphi_\infty - I_N \exp(iA_\infty s)\, \varphi_\infty \| = 0 \quad . \tag{3.14}$$

Let $\underline{\sigma}_N(t) = \exp(iH^S_N t)\, \underline{\sigma}_N \exp(-iH^S_N t)$ and $\alpha_N(t) = 2^{-1/2}(\xi_N(t) + i\pi_N(t))$. We shall prove in this section that

$$\xi_N(t) \xrightarrow{WT} \xi_t \ , \quad \pi_N(t) \xrightarrow{WT} \pi_t \ , \quad \underline{\sigma}_N(t) \xrightarrow{WT} \underline{\sigma}_t \ , \tag{3.15}$$

$$N^{1/2}(\xi_N(t) - \xi_t) \xrightarrow{WT} q_\infty(t) \ , \quad N^{1/2}(\pi_N(t) - \pi_t) \xrightarrow{WT} p_\infty(t) \ ,$$

$$N^{1/2}(\underline{\sigma}_N(t) - \underline{\sigma}_t) \xrightarrow{WT} \underline{s}_\infty(t) \quad . \tag{3.16}$$

Here α_t and $\underline{\sigma}_t$ satisfy the classical equations (2.9) with $\varkappa = \gamma = \delta = 0$ and initial conditions $(\alpha, \underline{\sigma})$ at $t = 0$. Clearly the classical equations have always global solutions, since $|\alpha|^2 + \sigma^3$ and $(\sigma^3)^2 + |\sigma^+|^2$ are invariant under the flow. $a_\infty(t)$ and $\underline{s}_\infty(t)$ are solutions of the linearized equations around the classical orbit :

$$\begin{aligned}
\dot{a}_\infty(t) &= -i\nu\, a_\infty(t) - i\lambda\, s^-_\infty(t) \ , \\
\dot{s}^-_\infty(t) &= -i\varepsilon\, s^-_\infty(t) + 2i\lambda \alpha_t\, s^3_\infty(t) + 2i\lambda \sigma^3_t\, a_\infty(t) \ , \\
\dot{s}^3_\infty(t) &= i\lambda (\alpha^*_t\, s^-_\infty(t) + \sigma^-_t\, a^*_\infty(t) - \text{h.c.}) \ ,
\end{aligned} \tag{3.17}$$

with initial conditions $a_\infty(0) = a_\infty$, $s_\infty(0) = s_\infty$.

Let $(\alpha, \underline{\sigma})$ be any initial state. Around the corresponding classical solution we develop H^S_N in powers of $N^{1/2}$ into a mean field

and a fluctuation part, $H_N^S = H_N^M(t) + H_N^F(t)$:

$$H_N^M(t) = \varepsilon S_N^3 + \lambda\alpha_t^- S_N^+ + \lambda\alpha_t^* S_N^- + N^{1/2}(\nu\alpha_t + \lambda\sigma_t^-)a^* +$$

$$+ N^{1/2}(\nu\alpha_t^* + \lambda\sigma_t^+)a - N(\nu\alpha_t^*\alpha_t + \lambda\alpha_t^*\sigma_t^- + \lambda\sigma_t^+\alpha_t) \qquad (3.18)$$

is well known from the thermodynamics of the BCS [T1] or of the Dicke model [H2], with an explicit time dependence, if the initial condition is not stationary. The action of $H_N^M(t)$ is purely group theoretical, a translation of the boson operators by the photon part and a rotation of the atomic observables. We shall see that $H_N^M(t)$ describes correctly the time-evolution of the intensive observables when $N \to \infty$.

$$H_N^F(t) = \nu(a^* - N^{1/2}\alpha_t^*)(a - N^{1/2}\alpha_t) + \lambda(a^* - N^{1/2}\alpha_t^*)N^{1/2}(\sigma_N^- - \sigma_t^-)$$

$$+ \lambda(a - N^{1/2}\alpha_t)N^{1/2}(\sigma_N^+ - \sigma_t^+) \qquad (3.19)$$

leads to nonlinear Heisenberg equations for the fluctuation operators, when $N < \infty$, which linearize for $N \to \infty$. Consider

$$U_N^M(t) = T \exp -i\int_0^t ds\, H_N^M(s) . \qquad (3.20)$$

Clearly this propagator exists for all t using a strongly convergent Dyson series on $\mathcal{H}_N^0$ and a unitary extension. $\hat{a}_N(t) = U_N^M(t)^*(a - N^{1/2}\alpha_t) \times U_N^M(t)$ satisfies $d\hat{a}_N(t)/dt = 0$ and $\hat{a}_N(0) = a - N^{1/2}\alpha$, hence

$$\hat{a}_N(t) = a - N^{1/2}\alpha . \qquad (3.21)$$

Similarly, $\hat{\underline{s}}_N(t) = U_N^M(t)^* N^{1/2}(\underline{s}_N - \underline{s}_t)U_N^M(t)$ satisfies

$$d\hat{s}_N^-(t)/dt = -i\varepsilon\hat{s}_N^-(t) + 2i\lambda\alpha_t\hat{s}_N^3(t) ,$$

$$d\hat{s}_N^3(t)/dt = -i\lambda\alpha_t\hat{s}_N^+(t) + i\lambda\alpha_t^*\hat{s}_N^-(t) , \qquad (3.22)$$

and has a global solution in terms of a 1-parameter family of rotations

$$\hat{\underline{s}}_N(t) = M(t)\, N^{1/2}(\underline{s}_N - \underline{s}) . \qquad (3.23)$$

Let us consider Weyl operators $W_N(t) = W_N(\alpha, \underline{\sigma}, t, x, y, \underline{z})$ of the form

$$W_N(\alpha,\underline{\mathfrak{T}},t,x,y,\underline{z}) = \exp i\left[x(q-N^{1/2}\xi_t)+y(p-N^{1/2}\pi_t)+\underline{z}(\underline{\mathfrak{T}}_N-\underline{\mathfrak{T}}_t)N^{1/2}\right]. \quad (3.24)$$

Then

$$\exp(iH_N^S t)\, W_N(t)\, \exp(-iH_N^S t) = \hat{V}_N(t,0)^* \hat{W}_N(t)\, \hat{V}_N(t,0) , \quad (3.25)$$

$$\hat{W}_N(t) = U_N^M(t)^* W_N(t)\, U_N^M(t) , \quad (3.26)$$

$$\hat{V}_N(t,0) = U_N^M(t)^* \exp(-iH_N^S t) . \quad (3.27)$$

$\hat{W}_N(t)$ is obtained from $W_N(t)$ by replacing in (3.24) $a-N^{1/2}\alpha_t$ by $a-N^{1/2}\alpha$ and $\underline{\mathfrak{T}}_N-\underline{\mathfrak{T}}_t$ by $M(t)(\underline{\mathfrak{T}}_N-\underline{\mathfrak{T}})$. $\hat{V}_N(t,0)$ is the solution of

$$d\hat{V}_N(t,0)/dt = -i\,\hat{H}_N^F(t)\,\hat{V}_N(t,0) , \quad \hat{H}_N^F(t) = U_N^M(t)^* H_N^F(t)\, U_N^M(t) . \quad (3.28)$$

The propagator

$$\hat{V}_N(t,s) = T \exp -i \int_s^t dr\, \hat{H}_N^F(r) \quad (3.29)$$

can again be defined by a Dyson series on $\mathcal{H}_N^0$, and $\hat{H}_N^F(r)$ is obtained from $H_N^F(r)$ by going over to fluctuation observables at time zero. Hence (3.29) can converge, when we pass to $N\to\infty$ along Ω_N .

Theorem 3.1 : For every physical initial condition α , $\underline{\mathfrak{T}}$ (with(3.3)), the intensive observables and the fluctuations along the classical orbit converge to (3.15) and (3.16) along $|\alpha,\underline{\mathfrak{T}}\rangle_N$ for $N\to\infty$.

Proof : For $|t-s|$ sufficiently small, the Dyson series for

$$\hat{V}_\infty(t,s) = T \exp -i \int_s^t dr\, \hat{H}_\infty^F(r) , \quad (3.30)$$

$$\hat{H}_\infty^F(r) = \gamma a_\infty^* a_\infty + \lambda(a_\infty^* s_\infty^-(r) + s_\infty^+(r) a_\infty) , \quad (3.31)$$

$$\underline{s}_\infty(r) = M(r)\, R\, \underline{t}_\infty , \quad (3.32)$$

converges in the strong topology on $\mathcal{H}_\infty^0$. Using (3.25) and the Schwarz inequality

$$\| I_N \hat{V}_\infty(t,0)^* \hat{W}_\infty(t)\, \hat{V}_\infty(t,0)\psi_\infty - \hat{V}_N(t,0)^* \hat{W}_N(t)\, \hat{V}_N(t,0)\, I_N \psi_\infty \| \leq$$

$$\leq \| I_N \hat{V}_\infty(t,0)^* \hat{W}_\infty(t) \hat{V}_\infty(t,0) \psi_\infty - \hat{V}_N(t,0)^* I_N \hat{W}_\infty(t) \hat{V}_\infty(t,0) \psi_\infty \| +$$

$$+ \| I_N \hat{W}_\infty(t) \hat{V}_\infty(t,0) \psi_\infty - \hat{W}_N(t) I_N \hat{V}_\infty(t,0) \psi_\infty \| +$$

$$+ \| I_N \hat{V}_\infty(t,0) \psi_\infty - \hat{V}_N(t,0) I_N \psi_\infty \| . \qquad (3.33)$$

For small $|t-s|$, the Duhamel formula can be used on $\mathcal{H}^0_\infty$:

$$\| I_N \hat{V}_\infty(t,s) \psi_\infty - \hat{V}_N(t,s) I_N \psi_\infty \| \qquad (3.34)$$

$$= \| i \int_s^t dr \, \hat{V}_N(t,r) \left[\hat{H}^F_N(r) I_N - I_N \hat{H}^F_\infty(r) \right] \hat{V}_\infty(r,s) \psi_\infty \|$$

$$\leq \int_s^t dr \, \| (\hat{H}^F_N(r) I_N - I_N \hat{H}^F_\infty(r)) \hat{V}_\infty(r,s) \psi_\infty \| ,$$

since the Dyson series for $\hat{V}_\infty(r,s)$ solves all domain problems. Hence (3.34) converges to zero for small $|t-s|$ and $\psi_\infty \in \mathcal{H}^0_\infty$, and therefore on all $\mathcal{H}_\infty$, since $\| I_N \| = \| \hat{V}_N(t,s) \| = \| \hat{V}_\infty(t,s) \| = 1$. Large $|t-s|$ can be estimated stepwise, e.g. $\| \hat{V}_N(t,0) I_N \psi_\infty - I_N \hat{V}_\infty(t,0) \psi_\infty \| \leq \| \hat{V}_N(s,0) I_N \psi_\infty - I_N \hat{V}_\infty(s,0) \psi_\infty \| + \| \hat{V}_N(t,s) I_N V_\infty(s,0) \psi_\infty - I_N V_\infty(t,0) \psi_\infty \|$. By expanding the exponential on any $\psi_\infty \in \mathcal{H}^0_\infty$, one proves that

$$\| I_N \hat{W}_\infty(t) \psi_\infty - \hat{W}_N(t) I_N \psi_\infty \| \longrightarrow 0 \quad \text{for} \quad N \longrightarrow \infty , \qquad (3.35)$$

and therefore on $\mathcal{H}_\infty$ by uniform boundedness. Hence all three terms on the r.h.s. of (3.33) go to zero for all t and all $\psi_\infty \in \mathcal{H}_\infty$. Now, $\hat{V}_\infty(t,0)^* \hat{W}_\infty(t) \hat{V}_\infty(t,0)$ has an exponential representation of the form (3.24) , where

$$a_\infty(t) = \hat{V}_\infty(t,0)^* \hat{a}_\infty(t) \hat{V}_\infty(t,0) ,$$

$$\underline{s}_\infty(t) = \hat{V}_\infty(t,0)^* \underline{\hat{s}}_\infty(t) \hat{V}_\infty(t,0) . \qquad (3.36)$$

One checks that (3.36) satisfies (3.17) with $a_\infty(0) = a_\infty$, $\underline{s}_\infty(0) = \underline{s}_\infty$, and by uniqueness the WT-convergence (3.16) follows. (3.15) can be derived similarly.

Corollary 3.2 : For all t_m, x_m, y_m, z_m, $1 \leq m \leq n$,

$$\lim_{N \to \infty} \left(\Omega_N, \prod_{m=1}^n \exp(iH^S_N t_m) \, W_N(\alpha, \underline{\beta}, t_m, x_m, y_m, z_m) \exp(-iH^S_N t_m) \, \Omega_N \right) =$$

$$= \left(\Omega_\infty, \prod_{m=1}^{n} W_\infty(\alpha, \underline{\xi}, t_m, x_m, y_m, z_m)\, \Omega_\infty\right) , \qquad (3.37)$$

and analogously for the intensive observables.

Proof : By repeated application of Theorem 3.1 one obtains WT-convergence for a product of time translated Weyl operators. This implies (3.37), since $\lim \left(I_N \varphi_\infty, I_N \psi_\infty\right) = (\varphi_\infty, \psi_\infty)$ by polarization.

It is typical for the classical limit of quantum mechanics in minimum uncertaincy states [H5] that the quantum mechanical correlation functions of intensive observables in coherent states (with amplitudes which are scaled so that the time zero expectation values converge) tend towards products of solutions of the classical equations, and that the fluctuations around the classical orbits follow linearized boson equations of motion. There is a close connection between the limit $N \to \infty$ and $\hbar$ fixed in mean field models and the limit $\hbar \to 0$ in ordinary quantum mechanics of a fixed number of degrees of freedom.

§4. The Lossy Laser

After having studied the classical limit for the closed system of atoms and radiation we shall now construct a model of a quantum mechanical reservoir with simple damping and pumping properties. A natural reservoir for photon losses in the laser is a quantized radiation field of infinitely many boson degrees of freedom, $a_w^\#$, which describes all the non-lasing photon modes of the world. The simplest interaction Hamiltonian is linear :

$$H^P = \int_{-\infty}^{+\infty} dw\, \varepsilon_w a_w^* a_w + \int_{-\infty}^{+\infty} dw\, k_w \left(a_w^* a + a^* a_w\right) , \qquad (4.1)$$

where for notational simplicity we take $w \in \mathbb{R}$ and a continuum normalization

$$\left[a_w , a_{w'}^*\right] = \delta(w-w') , \quad \left[a_w , a_{w'}\right] = 0 , \qquad (4.2)$$

Under the influence of H_N^S and H^P the Heisenberg equations become

$$\dot{a}_N(t) = -i\gamma\, a_N(t) - i\lambda\, S_N^-(t) N^{-1/2} - i \int_{-\infty}^{+\infty} k_w\, a_{wN}(t) , \qquad (4.3)$$

$$\dot{a}_{wN}(t) = -i\varepsilon_w a_{wN}(t) - ik_w a_N(t) . \qquad (4.4)$$

In the initial state we shall assume no correlations between the cavity and the reservoir, $\Omega_N = \Omega_N^S \otimes \Omega_N^R$, and take the photon reservoir to be empty, $a_w \Omega_N^R = 0$ for all w. A dissipation of the form (4.1) will in general not lead to phenomenological equations of the type (2.7) with a fluctuation force $g_N(t)$ independent of the state of the small system, unless the interaction with the reservoir is sufficiently "white" to destroy all memory effects. We can solve (4.4) for $a_{wN}(t)$ in terms of the initial condition a_w and $a_N(s)$ for $0 \leq s \leq t$, insert the solution into (4.3) and pass to the limit $k_w \to k$, $\varepsilon_w \to w$. This leads for $\alpha_N(t)$, $t \geq 0$, to

$$\dot{\alpha}_N(t) = -(i\gamma + \varkappa)\alpha_N(t) - i\lambda\sigma_N^-(t) + \chi_N(t) , \qquad (4.5)$$

where $\varkappa = \pi k^2$, $\chi_N(t) = -ikN^{-1/2}A(t)$ and where $A(t) = \int dw\, a_w\, e^{-iwt}$ is "white boson noise". Singular equations of motion of the type (4.5) require some care, but all the steps in the following, including some abusive notation, can be rigorously justified by treating H_N^R as a derivation and $\exp(iH_N^R t)(.)\exp(-iH_N^R t)$ as an automorphism of the Weyl and CAR algebra, which on a dense domain is defined by a convergent multicommutator series.

For the atomic degrees of freedom it is more complicated to find a phenomenologically acceptable and mathematically simple dissipation process. We shall couple the electrons of each atom to an electron sea of infinitely many degrees of freedom, again by a singular linear coupling :

$$H_N^A = \sum_{n=1}^{N} \sum_{\pm} H_{\pm n}^A , \qquad (4.6)$$

$$H_{\pm n}^A = \int_{-\infty}^{+\infty} dw\, w(b_{\pm nw}^* b_{\pm nw} + c_{\pm nw}^* c_{\pm nw}) + \int_{-\infty}^{+\infty} dw \left[b_{\pm n}^* (f_\pm b_{\pm nw} + g_\pm c_{\pm nw}) + h.c. \right]$$

using Fermi fields with normal anticommutation relations in continuum normalization (4.2). Under $H_N = H_N^S + H_N^A + H^P$, the time evolution of the atomic Fermi operators becomes

$$\dot{b}_{+n}(t) = -(i\varepsilon + \gamma)b_{+n}(t)/2 - i\lambda\alpha_N(t)b_{-n}(t) - if_+ B_{+n}(t) - ig_+ C_{+n}(t) , \qquad (4.7)$$

$$\dot{b}_{-n}(t) = -(\gamma - i\varepsilon)b_{-n}(t)/2 - i\lambda\alpha_N^*(t)b_{+n}(t) - if_-B_{-n}(t) - ig_-C_{-n}(t). \tag{4.8}$$

Here $B_{\pm n}(t) = \int dw\, b_{\pm nw} \exp(-iwt)$ and $C_{\pm n}(t)$ are "white fermion noise" operators and $\gamma = 2\pi(|g_+|^2 + |g_-|^2)$. We have assumed $|f_+|^2 + |g_+|^2 = |f_-|^2 + |g_-|^2$ and $|f_+|^2 = |g_-|^2$ in order to ensure macroscopic charge neutrality for the dissipation process, so that $\sum(b_{+n}^* b_{+n} + b_{-n}^* b_{-n})$ stays at N up to $N^{1/2}$ fluctuations.

The intensive observables obey the following differential equations

$$\dot{\sigma}_N^-(t) = -(i\varepsilon+\gamma)\,\sigma_N^-(t) + 2i\lambda\alpha_N(t)\sigma_N^3(t) + \varphi_N^-(t), \tag{4.9}$$

where the fluctuation force $\varphi_N^-(t) = \varphi_N^+(t)^*$ unfortunately depends on the observables of the small system:

$$\varphi_N^+(t) = \varphi_N^{++}(t) + \varphi_N^{+-}(t), \tag{4.10}$$

$$\varphi_N^{++}(t) = iN^{-1}\sum_{n=1}^{N}\left[f_+^* B_{+n}^*(t)b_{-n}(t) + g_-C_{-n}(t)b_{+n}(t)\right], \tag{4.11}$$

$$\varphi_N^{+-}(t) = -iN^{-1}\sum_{n=1}^{N}\left[f_-b_{+n}^*(t)B_{-n}(t) + g_+^* b_{-n}(t)C_{+n}^*(t)\right].$$

Similarly

$$\dot{\sigma}_N^3(t) = -\gamma(\sigma_N^3(t) - \eta) + i\lambda\alpha_N^*(t)\sigma_N^-(t) - i\lambda\alpha_N(t)\sigma_N^+(t) + \varphi_N^3(t), \tag{4.12}$$

$$\varphi_N^3(t) = \varphi_N^{3+}(t) + \varphi_N^{3-}(t), \quad \varphi_N^{3-}(t) = \varphi_N^{3+}(t)^*, \tag{4.13}$$

$$\varphi_N^{3+}(t) = (2N)^{-1}\sum_{n=1}^{N}\left[ig_+C_{+n}(t)b_{+n}^*(t) - ig_-C_{-n}(t)b_{-n}^*(t) + \right.$$

$$\left. + if_+^* B_{+n}^*(t)b_{+n}(t) - if_-^* B_{-n}^*(t)b_{-n}(t)\right]. \tag{4.14}$$

In (4.12) the "unsaturated inversion" $\eta = \pi\gamma^{-1}(|g_+|^2 - |g_-|^2)$ was split off, in order to obtain for $i = \pm, 3$

$$\varphi_N^{i-}(t)\,\Omega_N^R = \varphi_N^{i+}(t)^*\,\Omega_N^R = 0, \tag{4.15}$$

if the B-reservoir is empty, $B_{+n}(t)\,\Omega_N^R = 0$, and the C-reservoir full, $C_{+n}^*(t)\,\Omega_N^R = 0$. By a suitable choice of $|g_\pm|^2$, we can reach any $-1/2 \le \eta \le 1/2$.

By generalizing the approach of Section 3 we shall study the WT convergence of the intensive and fluctuation observables along $\Omega_N = \Omega_N^S \otimes \Omega_N^R$, where Ω_N^R is the vacuum of the reservoir fields and Ω_N^S is coherent, $\Omega_N^S = |\alpha, \underline{\sigma}\rangle_N$. Given any physical initial condition $\alpha, \underline{\sigma}$, we split H_N along the classical orbit $\alpha_t, \underline{\sigma}_t$ into a mean field and a fluctuation part, $H_N = H_N^M(t) + H_N^F(t)$:

$$H_N^M(t) = H^P + \gamma a^* a + \lambda N^{1/2}(a^* \sigma_t^- + \sigma_t^+ a) + \tag{4.16}$$

$$+ H_N^A + \varepsilon S_N^3 + \lambda(\alpha_t S_N^+ + \alpha_t^* S_N^-) - N(\alpha_t^* \sigma_t^- + \sigma_t^+ \alpha_t) ,$$

$$H_N^F(t) = \lambda(a^* - N^{1/2}\alpha_t^*) N^{1/2}(\sigma_N^- - \sigma_t^-) + \text{h.c.} \tag{4.17}$$

Under $H_N^M(t)$ the photons and the different atoms are uncoupled. Since the initial state is a product state with strong factorization properties, this will lead to "boson white noise" fluctuation forces for the fluctuation observables, when $N \to \infty$. In the corresponding interaction picture, $\hat{H}_N^F(t)$ will again become quadratic in boson operators. We will study the evolution of Weyl operators (3.24) which can be represented in the form (3.25,26,27) with H_N^S replaced by H_N and with $U_N^M(t)^*(.)U_N^M(t)$ considered as an automorphism. We compute $\hat{a}_N(t)$ and $\hat{s}_N(t)$ from their differential equations :

$$d\hat{a}_N(t)/dt = - (i\gamma + \varkappa)\hat{a}_N(t) - ik\, A(t) ,$$

$$\hat{a}_N(t) = \exp-(i\gamma + \varkappa)t\ (a - N^{1/2}\alpha) - ik \int_0^t ds\ A(s)\ \exp-(i\gamma + \varkappa)(t-s) , \tag{4.18}$$

$$d\hat{s}_N^-(t)/dt = - (i\varepsilon + \gamma)\hat{s}_N^-(t) + 2i\lambda\alpha_t \hat{s}_N^3(t) + f_N^-(t) ,$$

$$d\hat{s}_N^3(t)/dt = - \gamma \hat{s}_N^3(t) + i\lambda\alpha_t^* \hat{s}_N^-(t) - i\lambda\alpha_t \hat{s}_N^+(t) + f_N^3(t) . \tag{4.19}$$

In terms of the propagator $P(t,s)$ of (4.19) one has

$$\hat{\underline{s}}_N(t) = P(t,0) N^{1/2}(\underline{\sigma}_N - \underline{\sigma}) + \int_0^t ds\ P(t,s)\ \underline{f}_N(s) . \tag{4.20}$$

In (4.19), the fluctuation forces $\underline{f}_N(t) = \underline{f}_N^+(t) + \underline{f}_N^-(t)$ satisfy

$$\underline{f}_N^{\pm}(t) = M^{-1/2} \sum_{m=1}^{M} \hat{f}_m^{\pm}(t) , \quad \hat{f}_m^{\pm}(t) = (2p+q)^{-1/2} \sum_{n \in \Delta(m)} F_n^{\pm}(t) , \tag{4.21}$$

where $\Delta(m) = [(2p+q)m, (2p+q)(m+1)]$. The $F_n^{\pm}(t)$ have the form (4.10,11,13,14) without N^{-1} and $\sum_{n=1}^{N}$ and with the $b_{\pm n}(t)$ evolved under $H_N^M(t)$. The $b_{\pm n}(t)$ therefore obey (4.7,8) with $\alpha_N(t)$ replaced by the c-number α_t and, as a consequence of the direct product structure of Ω_N, one has for all $1 \le m \le M$

$$\begin{aligned}(2p+q)^{-1} \sum_{n \in \Delta(m)} (\Omega_N, b_{+n}^*(t) b_{-n}(t)\, \Omega_N) &= \sigma_t^+ , \\ (2p+q)^{-1} \sum_{n \in \Delta(m)} (\Omega_N, (b_{+n}^*(t) b_{+n}(t) - b_{-n}^*(t) b_{-n}(t))\Omega_N) &= 2\sigma_t^3 ,\end{aligned} \tag{4.22}$$

where the σ_t^i satisfy the classical equations (2.9). Hence the correlation functions in $(\Omega_N, \cdot\, \Omega_N) = \langle \cdot \rangle_N$ are δ-correlated and independent of m :

$$\begin{aligned}\langle \hat{f}_m^-(s) \hat{f}_m^-(t) \rangle_N &= \langle \hat{f}_m^+(s) \hat{f}_m^+(t) \rangle_N = 0 \\ \langle \hat{f}_m^-(s) \hat{f}_m^+(t) \rangle_N &= \delta(s-t)\, \gamma(1/2 - \eta)(1 - 2\sigma_t^3) \\ \langle \hat{f}_m^3(s) \hat{f}_m^3(t) \rangle_N &= \delta(s-t)\, \gamma(1/4 + \eta\sigma_t^3) \\ \langle \hat{f}_m^3(s) \hat{f}_m^+(t) \rangle_N &= \langle \hat{f}_m^3(s) \hat{f}_m^-(t) \rangle_N^* = \delta(s-t)\, \gamma(1/2 - \eta)\sigma_t^+ \\ \langle \hat{f}_m^+(s) \hat{f}_m^3(t) \rangle_N &= \langle \hat{f}_m^-(s) \hat{f}_m^3(t) \rangle_N^* = -\delta(s-t)\, \gamma(1/2 + \eta)\sigma_t^+\end{aligned} \tag{4.23}$$

Furthermore, since $\hat{f}_m^-(t)\Omega_N = \hat{f}_m^+(t)^* \Omega_N = 0$ and $[\hat{f}_m^{\pm}(s), \hat{f}_n^{\pm}(t)] = 0$ for $m \neq n$, one has independent of $N = M(2p+q)$

$$\langle f_N^i(s) f_N^j(t) \rangle_N = \langle \hat{f}_m^i(s) \hat{f}_m^j(t) \rangle_N \tag{4.24}$$

The 2-point function of $\hat{f}_m^i(s)$ with $A^{\#}(t)$ or any fluctuation operator at $t = 0$ vanishes. However, the higher correlation funtions of such quantities are far from Gaussian for finite N.

Let $\mathcal{H}_\infty$ be the Fock space of two boson modes $a_\infty^{\#}$ and $t_\infty^{\pm}$ and four boson fields $A_\infty^{\#}(t)$, $f_\infty^{i+}(t)$, $i=1,2,3$, with test function space $L^2([0,\infty))$ and cyclic vacuum Ω_∞, satisfying

$$f_\infty^{i-}(t)\Omega_\infty = a_\infty \Omega_\infty = A_\infty(t)\Omega_\infty = t_\infty^- \Omega_\infty = 0 \tag{4.25}$$

$$f_{\infty}^{i+}(t) = f_{\infty}^{i-}(t)^*, \; t_{\infty}^{+} = t_{\infty}^{-*}, \; f_{\infty}^{\pm\pm}(t) = f_{\infty}^{1\pm}(t) \pm i f_{\infty}^{2\pm}(t) ,$$

and with c-number commutators, which all vanish except for

$$[a_{\infty}, a_{\infty}^*] = 1, \quad [t_{\infty}^{-}, t_{\infty}^{+}] = 2\sigma , \quad [f_{\infty}^{i-}(s), f_{\infty}^{j+}(t)] = \langle f_N^i(s) f_N^j(t) \rangle_N . \tag{4.26}$$

The identification mapping $I_N : \mathcal{H}_{\infty} \to \mathcal{H}_N$ is defined by linear extension of

$$I_N \, a_{\infty}^{*i} A_{\infty}^*(s_1) .. A_{\infty}^*(s_j) (t_{\infty}^{+})^k f_{\infty}^{n_1+}(t_1) .. f_{\infty}^{n_r\pm}(t_r) \, \Omega_{\infty} = \tag{4.27}$$

$$= M^{-(k+r)/2} \sum\nolimits' (a^* - N^{1/2}\alpha^*)^i A^*(s_1) .. A^*(s_j) \hat{t}_{m_1}^{+} .. \hat{t}_{m_k}^{+} \hat{f}_{m_{k+1}}^{n_1+}(t_1) .. \hat{f}_{m_{k+r}}^{n_r\pm}(t_r) \, \Omega_N .$$

where $\sum'$ extends over all $m_1, \ldots m_{k+r} = 1, .. M$ with $m_k \neq m_l$ for $k \neq l$, and $t_N^{+} = M^{-1/2} \sum_{m=1}^{M} \hat{t}_m^{+}$ as in (4.21). Let $\mathcal{H}_{\infty}^h \subset \mathcal{H}_{\infty}$ be the span of all vectors of the type (4.27) with $k + r = h$. Because of the product struture of Ω_N there exists an isometry I_N^h such that

$$I_N \restriction \mathcal{H}_{\infty}^h = \prod_{g=1}^{h-1} (1 - g/M)^{1/2} \, I_N^h \tag{4.28}$$

Hence $\| I_N \| = 1$ and $\lim_{N\to\infty} \| I_N \varphi_{\infty} \| = \| \varphi_{\infty} \|$ for all $\varphi_{\infty} \in \mathcal{H}_{\infty}$. Now, we are ready to prove the main theorem on the time evolution of the laser :

Theorem 4.1 : In the DHL model (2.4), (4.1,6) the intensive observables $\alpha_N(t)$, $\underline{\sigma}_N(t)$ converge in the WT sense along $\Omega_N = |\alpha, \underline{\sigma}\rangle_N \otimes \Omega_N^R$ (with (3.3)) towards the solutions α_t, $\underline{\sigma}_t$ of the classical equations (2.9) with initial conditions $\alpha_0 = \alpha$, $\underline{\sigma}_0 = \underline{\sigma}$. The fluctuation operators $a_N(t) = N^{1/2}(\alpha_N(t) - \alpha_t)$, $\underline{s}_N(t) = N^{1/2}(\underline{\sigma}_N(t) - \underline{\sigma}_t)$ converge in the WT sense towards solutions $a_{\infty}(t)$, $\underline{s}_{\infty}(t)$ in $\mathcal{H}_{\infty}$ of the linearized equations

$$\dot{a}_{\infty}(t) = -(i\gamma + \varkappa) a_{\infty}(t) - i\lambda s_{\infty}^{-}(t) - ik \, A_{\infty}(t) , \tag{4.29}$$

$$\dot{s}_{\infty}^{-}(t) = -(i\varepsilon + \gamma) s_{\infty}^{-}(t) + 2i\lambda \alpha_t s_{\infty}^{3}(t) + 2i\lambda \sigma_t^{3} a_{\infty}(t) + f_{\infty}^{-}(t) ,$$

$$\dot{s}_{\infty}^{3}(t) = -\gamma s_{\infty}^{3}(t) + i\lambda (\alpha_t^* s_{\infty}^{-}(t) + \sigma_t^{-} a_{\infty}^*(t) - \text{h.c.}) + f_{\infty}^{3}(t) ,$$

with $t \geq 0$ and initial condition $a_{\infty}(0) = a_{\infty}$, $\underline{s}_{\infty}(0) = \underline{s}_{\infty}$ in $\mathcal{H}_{\infty}$. Also the correlation functions converge in the sense of (3.37).

Proof : As in theorem 3.1, we consider the Weyl operators

$$\exp(iH_N t)\, W_N(\alpha,\underline{\xi},t,x,y,z)\, \exp(-iH_N t) = \hat{V}_N(t,0)^* \hat{W}_N(t) \hat{V}_N(t,0) \,. \qquad (4.30)$$

Here $\hat{W}_N(t) = \exp(i\hat{K}_N(t))$ is obtained from (3.24) by replacing $a - N^{1/2}\alpha_t$ by $\hat{a}_N(t)$ and $N^{1/2}(\underline{\xi}_N - \underline{\xi}_t)$ by $\underline{\hat{s}}_N(t)$, which gives a rigorous meaning to the l.h.s. of (4.30). $\hat{V}_N(t,s) = T \exp -i\int_s^t dr\, \hat{H}_N^F(r)$ is defined by a Dyson series with the same substitution as in $\hat{W}_N(t)$. The estimate (3.33) proves convergence, if we can show for $0 \le u \le 1$ and $0 \le s \le r \le t$ with $|t-s|>0$ sufficiently small and for every $\psi_\infty \in \mathcal{K}_\infty^0$ that

$$\begin{aligned} &\| (I_N \hat{H}_\infty^F(r) - \hat{H}_N^F(r) I_N) \hat{V}_\infty(r,s)\, \psi_\infty \| \,, \\ &\| (I_N \hat{K}_\infty(t) - \hat{K}_N(t) I_N) \exp(iu\hat{K}_\infty(t))\, \psi_\infty \| \end{aligned} \qquad (4.31)$$

are uniformly bounded in N and converge to zero for every r,u, if $N \to \infty$. Here $\hat{H}_\infty^F(r)$, $\hat{K}_\infty(t)$ and $\hat{V}_\infty(r,s)$ are analogously defined using $\hat{a}_\infty(t)$ and $\underline{\hat{s}}_\infty(t)$, the I_N-preimages of (4.18) and (4.20). The uniform boundedness and convergence of (4.31) can be easily proved by expanding $\hat{V}_\infty(r,s)\psi_\infty$ and $\exp(iu\hat{K}_\infty(t))\psi_\infty$ and by using (4.28). The limits $a_\infty(t) = \hat{V}_\infty(t,0)^* \hat{a}_\infty(t) \hat{V}_\infty(t,0)$ and $\underline{s}_\infty(t)$ are identified by the differential equation (4.29) which they satisfy.

§5. Conclusion

We have discussed in considerable detail a microscopic quantum mechanical model for a laser cavity coupled to different reservoirs and have given a precise sense in which the laser shows irreversible classical and stochastic behavior in the thermodynamic limit. We have, however, only barely prodded the sleeping giant of nonequilibrium statistical mechanics. There are many open problems in this field, both of a technical and conceptual nature. There is the immediate question, whether the choice of the reservoirs, in particular the use of regular Hamiltonians and nonlinear couplings, can qualitatively change the phase transition in this class of mean field models. A nontrivial generalization of our approach is necessary in order to treat the finite mode laser. Our results on the intensive and fluc-

tuation observables are the first two terms in an asymptotic expansion for large finite lasers. It is not clear how good this expansion is, if one is interested in the equilibrium properties of the finite nonlinear system for $t \to \infty$. Hopefully, the two limits, $N \to \infty$ and $t \to \infty$, can be exchanged for certain observables away from threshold. Finally, it is clear that the really hard problems of irreversible statistical mechanics are not the construction of quantum mechanical cuckoo clocks but the understanding of continuous systems with short range and Coulomb forces.

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THE LASER: A REVERSIBLE QUANTUM DYNAMICAL SYSTEM WITH IRREVERSIBLE CLASSICAL MACROSCOPIC MOTION

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We shall describe a mathematical machine which behaves like a laser but which, admittedly, is much simpler than any laser found in the laboratory. Our machine will consist of two main parts: the first one, which is the laser proper, consists of atoms and photons which are the quantized proper vibrations of a resonant cavity. It is essential that the number, N, of atoms be allowed to become very large, but the number of different photon modes can be infinite or finite. This number can in fact be one in order for the machine to operate, but in real life the number of modes is infinite. We can handle the infinite mode case provided that essentially only a finite number of modes is macroscopically excited. As the one-mode case is simpler, we shall mainly discuss it.

The second part consists of reservoirs. They are dynamical systems which in some sense are infinitely large compared to N, and they are so constructed that they can both pump energy into and drain energy out of the laser. The main point, however, is that the energy flux from reservoir to laser is thoroughly chaotic. The interesting property of the laser is that it can take this energy and structure it. In other words, the laser, when suitably coupled to the reservoir, will go into a cooperative oscillatory state in which all the N atoms and the photons vibrate coherently and periodically. In this regard the laser behaves like a clock or a steam engine or a scientists's brain.

To describe the operation of our machine we first have to show how each component operates separately. The analysis has several parts: one is the quantum mechanical level; another is the $N \to \infty$ limit in which the quantum equations go over into ordinary classical differential equations which, being nonlinear, have interesting bifurcation properties; a third level is the analysis of the quantum fluctuations around the classical orbit.

1. THE ATOMS

What we basically want to have for an atom is a very anharmonic oscillator. While one could possibly construct a laser with classical oscillators as "atoms", there exist quantum mechanical systems which quite naturally fulfill our requirements, namely two-level atoms. Each atom has two levels, each of which can either be occupied or not by one electron. Thus, there are four possible states for an atom. This is described by a four dimensional (complex) vector space, $\mathcal{V} = \mathcal{V}_+ \otimes \mathcal{V}_-$, where $\mathcal{V}_+$ (resp. $\mathcal{V}_-$) is a two-dimensional space for the upper (resp. lower) level. As an orthogonal basis in $\mathcal{V}_+$ (resp. $\mathcal{V}_-$) we take e_+^0 and e_+^1 (resp. e_-^0 and e_-^1) where 0 stands for unoccupied and 1 for occupied.

As generators for the operator algebra on $\mathcal{V}_+$, we take b_+, b_+^* and I, where

$$b_+ e_+^1 = e_+^0 \ , \ b_+ e_+^0 = 0 \ . \tag{1}$$

Note: the superscript * will always mean adjoint when referring to operators or complex conjugate when referring to numbers. b_+ is called the annihilation operator and b_+^* the creation operator. Likewise, we have $b_-^\# = b_-$, b_-^* for $\mathcal{V}_-$. A particularly important subspace $\mathcal{W}$ of $\mathcal{V}$ is the one spanned by $e_+^1 \otimes e_-^0$ and $e_+^0 \otimes e_-^1$. In $\mathcal{W}$, each atom has exactly one electron. On $\mathcal{W}$, the operators

$$\begin{aligned} S^+ &= b_+^* b_- = (S^-)^* \\ S^3 &= \frac{1}{2}(b_+^* b_+ - b_-^* b_-) = \frac{1}{2}[S^+, S^-] \end{aligned} \tag{2}$$

form an irreducible representation of SU(2) with spin 1/2. The Hilbert space $\mathcal{H}^A_{(N)}$ for N atoms is the N-fold tensor product of $\mathcal{V}$. Let $\varepsilon > 0$. The Hamiltonian

$$H^A_{(N)} = \varepsilon \, S^3_{(N)} \equiv \varepsilon \sum_{n=1}^{N} S^3_n \tag{3}$$

measures the total energy of the electrons when the values $\pm \varepsilon/2$ are given to the upper and lower level. Note that the subscript n labels the atoms. Under the unitary transformation $A \to A(t) = \exp(i H^A_{(N)} t) A \exp(-i H^A_{(N)} t)$ the $S^i_n(t)$ satisfy the Heisenberg equations of motion

$$\dot{S}^3_n(t) \equiv \frac{d}{dt} S^3_n(t) = 0 \ , \tag{4}$$

$$\dot{S}^+_n(t) = i \varepsilon \, S^+_n(t) \ . \tag{5}$$

We conclude our introduction to quantum mechanics by mentioning the concept of a state. For N finite, a state of the atomic system is described by a density matrix, i.e., a positive operator, $\omega_{(N)}$ on $\mathcal{H}^A_{(N)}$ with trace one. The expectation value of an observable, i.e., of an operator A on $\mathcal{H}^A_{(N)}$, in the state $\omega_{(N)}$ is given by

$$\omega_{(N)}(A) = \mathrm{Tr}\, A\omega_{(N)} \tag{6}$$

A pure state is a $\omega_{(N)}$ which is a one-dimensional projection onto a normalized vector $\psi \in \mathcal{H}^{A}_{(N)}$, i.e.,

$$\omega_{(N)}(A) = (\psi, A\psi) \tag{7}$$

for pure states.

2. THE RADIATION FIELD (PHOTONS)

The atoms are in a three-dimensional cavity which is a box of length L. The free classical electromagnetic field with periodic boundary condition has normal modes of vibration, called photons, of the form $\exp i(\underset{\sim}{k}.\underset{\sim}{x} - |\underset{\sim}{k}|t)$, where the vector $\underset{\sim}{k} \in \Gamma(L) = \left\{ \frac{2\pi}{L} \underset{\sim}{n} \mid \underset{\sim}{n} \in \mathbb{Z}^3 \right\}$. We neglect the fact that the photons have a polarization. If $a(\underset{\sim}{k})$ is the amplitude of the $\underset{\sim}{k}$-th mode, the total energy (in proper units, such that $\hbar = c = 1$) of the field is

$$H^{P}_{(L)} = \sum_{\underset{\sim}{k} \in \Gamma(L)} |\underset{\sim}{k}|\, a^{*}(\underset{\sim}{k})\, a(\underset{\sim}{k}) \tag{8}$$

In a fully quantum theory, the electromagnetic field should be quantized. This means that $a(\underset{\sim}{k})$, instead of being a complex number, is an operator on a Hilbert space $\mathcal{H}^{P}_{(L)}$ and satisfies the canonical commutation relations

$$[a(\underset{\sim}{k}), a^{*}(\underset{\sim}{q})] = \delta_{\underset{\sim}{k},\underset{\sim}{q}}, \quad [a(\underset{\sim}{k}), a(\underset{\sim}{q})] = 0 \tag{9}$$

where δ is the Kronecker delta. $\mathcal{H}^{P}_{(L)}$, the Fock space, is the span of all vectors $a^{*}(\underset{\sim}{k}_1) \ldots a^{*}(\underset{\sim}{k}_n)\, \Omega^{P}$, where Ω^{P}, the photon vacuum state, satisfies

$$a(\underset{\sim}{k})\, \Omega^{P} = 0 \text{ for all } \underset{\sim}{k} \in \Gamma(L). \tag{10}$$

In $\mathcal{H}^{P}_{(L)}$, $H^{P}_{(L)}$ is an unbounded self-adjoint operator. As a consequence of (9) the $a_{(L)}(\underset{\sim}{k},t) \equiv \exp(iH^{P}_{(L)}t)\, a(\underset{\sim}{k}) \exp(-iH^{P}_{(L)}t)$ satisfy Maxwell's equations

$$a_{(L)}(\underset{\sim}{k},t) = -i|\underset{\sim}{k}|\, a_{(L)}(\underset{\sim}{k},t), \tag{11}$$

and they are the unique solutions of (11) with $a_{(L)}(\underset{\sim}{k},0) = a(\underset{\sim}{k})$ on the domain of $H^{P}_{(L)}$[1].

3. THE ATOM-FIELD INTERACTION

To begin with, we shall henceforth assume that $L^3 = N \in \mathbb{Z}_+$ and use N instead of L(N) as a label for the cavity. The atoms are regarded as being distributed inside the cavity with small density fluctuations for $N \to \infty$ and $\underset{\sim}{x}_n \in \mathbb{R}^3$ is the coordinate of the n-th atom.

The Hilbert space $\mathscr{H}^S_{(N)}$ for the laser proper, i.e., for N atoms in a cavity of length L(N), is $\mathscr{H}^A_{(N)} \otimes \mathscr{H}^P_{(N)}$. The Hamiltonian has the form

$$H_{(N)} = H^A_{(N)} + H^P_{(N)} + H^{AP}_{(N)} \tag{12}$$

where $H^A_{(N)}$ and $H^P_{(N)}$ are as before [(3) and (8)] and

$$H^{AP}_{(N)} = N^{-1/2} \sum_{k \in \Gamma(N)} \sum_{n=1}^{N} \left\{ e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}_n} a(\underset{\sim}{k}) \, [\lambda(\underset{\sim}{k}) S^+_n + \mu(\underset{\sim}{k}) S^-_n] \right. \tag{13}$$

$$\left. + e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}_n} a^*(\underset{\sim}{k}) \, [\lambda^*(\underset{\sim}{k}) \, S^-_n + \mu^*(\underset{\sim}{k}) \, S^+_n] \right\} ,$$

where $\lambda(\underset{\sim}{k})$ and $\mu(\underset{\sim}{k})$ are continuous functions on $\mathbb{R}^3$ with rapid decrease at infinity. This interaction Hamiltonian is a well known [2] and reasonable approximation to quantum electrodynamics and we shall not try to justify it here. Physically, one usually has that $|\lambda(\underset{\sim}{k})| = |\mu(\underset{\sim}{k})|$, but we shall not assume this. In fact, it is often mathematically convenient and physically justified to suppose that $\mu(\underset{\sim}{k}) = 0$. This is called the rotating wave approximation to quantum electrodynamics. It leads to the conservation law that the operator

$$C_{(N)} = \sum_{\underset{\sim}{k} \in \Gamma(N)} a^*(\underset{\sim}{k}) \, a(\underset{\sim}{k}) + S^3_{(N)} \tag{14}$$

commutes with $H_{(N)}$.

Using $H_{(N)}$, one easily computes the new Heisenberg equations of motion to be

$$\dot{a}_{(N)}(\underset{\sim}{k},t) = -i|\underset{\sim}{k}|a_{(N)}(\underset{\sim}{k},t) - iN^{-1/2}\left\{\lambda^*(\underset{\sim}{k})\, S^-_{(N)}(-\underset{\sim}{k},t) + \mu^*(\underset{\sim}{k})S^+_{(N)}(-\underset{\sim}{k},t)\right\}$$

$$\dot{S}^-_{(N)}(\underset{\sim}{k},t) = -i\varepsilon S^-_{(N)}(\underset{\sim}{k},t) + 2iN^{-1/2}\sum_{\underset{\sim}{q}\in\Gamma(N)}\left\{\lambda(\underset{\sim}{q})a_{(N)}(\underset{\sim}{q},t)\cdot S^3_{(N)}(\underset{\sim}{k}+\underset{\sim}{q},t)\right.$$

$$\left. + \mu^*(\underset{\sim}{q})\, a^*_{(N)}(\underset{\sim}{q},t)\, S^3_{(N)}(\underset{\sim}{k}-\underset{\sim}{q},t)\right\} \tag{15}$$

$$\dot{S}^3_{(N)}(\underset{\sim}{k},t) = iN^{-1/2}\sum_{\underset{\sim}{q}\in\Gamma(N)}\left\{\mu(\underset{\sim}{q})\, a_{(N)}(\underset{\sim}{q},t)\, S^-_{(N)}(\underset{\sim}{k}+\underset{\sim}{q},t)\right.$$

$$+ \lambda^*(\underset{\sim}{q})\, a^*_{(N)}(\underset{\sim}{q},t)\, S^-_{(N)}(\underset{\sim}{k}-\underset{\sim}{q},t) - \mu^*(\underset{\sim}{q})\, a^*_{(N)}(\underset{\sim}{q},t)$$

$$\left.\cdot\, S^+_{(N)}(\underset{\sim}{k}-\underset{\sim}{q},t) - \lambda(\underset{\sim}{q})\, a_{(N)}(\underset{\sim}{q},t)\, S^+_{(N)}(\underset{\sim}{k}+\underset{\sim}{q},t)\right\}.$$

Here we have introduced for $i \in \{+,-,3\}$ the notation

$$S^i_{(N)}(\underset{\sim}{k},t) = \sum_{n=1}^{N} e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}_n}\, S^i_n(t)\,. \tag{16}$$

4. PROPERTIES OF THE EQUATIONS OF MOTION

The equations (15) are nonlinear operator differential equations which have unique global solutions on the domain of $H_{(N)}$, which is the domain of $H^p_{(N)}$. To understand their physical content it is helpful to keep track of the powers of N in (15). The intensive observables

$$\sigma^i_{(N)}(\underset{\sim}{k},t) = N^{-1} S^i_{(N)}(\underset{\sim}{k},t)$$

$$\alpha_{(N)}(\underset{\sim}{k},t) = N^{-1/2} a_{(N)}(\underset{\sim}{k},t) \tag{17}$$

satisfy the equations of motion

$$\dot{\alpha}(\underset{\sim}{k},t) = -i|\underset{\sim}{k}|\,\alpha(\underset{\sim}{k},t) - i\lambda^*(\underset{\sim}{k})\,\sigma^-(-\underset{\sim}{k},t) - i\mu^*(\underset{\sim}{k})\,\sigma^+(-\underset{\sim}{k},t)$$

$$\dot{\sigma}^-(\underset{\sim}{k},t) = -i\varepsilon\sigma^-(\underset{\sim}{k},t) + 2i\sum_{\underset{\sim}{q}} \Big\{\lambda(\underset{\sim}{q})\,\alpha(\underset{\sim}{q},t)\,\sigma^3(\underset{\sim}{k}+\underset{\sim}{q},t) + \mu^*(\underset{\sim}{q})\,\alpha^*(\underset{\sim}{q},t)\,\sigma^3(\underset{\sim}{k}-\underset{\sim}{q},t)\Big\} \tag{18}$$

$$\dot{\sigma}^3(\underset{\sim}{k},t) = i\sum_{\underset{\sim}{q}} \Big\{\mu(\underset{\sim}{q})\,\alpha(\underset{\sim}{q},t)\,\sigma^-(\underset{\sim}{k}+\underset{\sim}{q},t) + \lambda^*(\underset{\sim}{q})\,\alpha^*(\underset{\sim}{q},t)\,\sigma^-(\underset{\sim}{k}-\underset{\sim}{q},t) - \mu^*(\underset{\sim}{q})\,\alpha^*(\underset{\sim}{q},t)\,\sigma^+(\underset{\sim}{k}-\underset{\sim}{q},t) - \lambda(\underset{\sim}{q})\,\alpha(\underset{\sim}{q},t)\,\sigma^+(\underset{\sim}{k}+\underset{\sim}{q},t)\Big\}.$$

We have suppressed the index N, since we shall see immediately that in a suitable topology the operators $\sigma^i_{(N)}(\underset{\sim}{k},t)$ and $\alpha_{(N)}(\underset{\sim}{k},t)$ (which have equal time commutators bounded by $1/N$) will converge towards complex number valued functions $\sigma^i(\underset{\sim}{k},t)$ and $\alpha(\underset{\sim}{k},t)$, which are solutions of the equations of motion (18) considered as classical dynamical equations.

For this limit we must, however, restrict the modes coupled in (18) to belong to a fixed cavity M and sum over $\underset{\sim}{q} \in \Gamma(M)$. We assume that

$\lambda(\underset{\sim}{0}) = \mu(\underset{\sim}{0}) = 0$ and that $\sum_{\underset{\sim}{k} \in \Gamma(M)} \{|\lambda(\underset{\sim}{k})| + |\mu(\underset{\sim}{k})|\} < \infty$.

Let $\mathscr{G}^M$ be the Hilbert space of all sequences

$$\rho = \{\rho^i\}_{i=1}^{\infty} \equiv \{\alpha(\underset{\sim}{k}) \in \mathbb{C},\ \sigma^+(\underset{\sim}{k}) = \sigma^-(-\underset{\sim}{k})^*,$$

$$\sigma^3(\underset{\sim}{k}) = \sigma^3(-\underset{\sim}{k})^* \in \mathbb{C} \mid \underset{\sim}{k} \in \Gamma(M)\} \quad , \tag{19}$$

with

$$\|\rho\|^2 = \sum_{\underset{\sim}{k} \in \Gamma(M)} \{|\alpha(\underset{\sim}{k})|^2 + |\sigma^+(\underset{\sim}{k})|^2 + |\sigma^3(\underset{\sim}{k})|^2\} < \infty \tag{20}$$

$\mathscr{G}^M$ is the classical phase space for our system. For every initial condition $\rho \in \mathscr{G}^M$, the classical equations (18) have global unique solutions. For small t, this follows by the contraction mapping theorem. Quantities invariant under the flow are

$$\begin{aligned} h &= \sum_{\underset{\sim}{k} \in \Gamma(M)} |\underset{\sim}{k}|\ |\alpha(\underset{\sim}{k})|^2 + \varepsilon\, \sigma^3(\underset{\sim}{0}) \\ &+ \sum_{\underset{\sim}{k} \in \Gamma(M)} \{\alpha(\underset{\sim}{k})\ (\lambda(\underset{\sim}{k})\sigma^+(\underset{\sim}{k}) + \mu(\underset{\sim}{k})\ \sigma^-(\underset{\sim}{k}) + \text{c.c.}\} \quad , \\ s &= \sum_{\underset{\sim}{k} \in \Gamma(M)} \{|\sigma^+(\underset{\sim}{k})|^2 + |\sigma^3(\underset{\sim}{k})|^2\} \quad . \end{aligned} \tag{21}$$

Since $\lambda(\underset{\sim}{0}) = \mu(\underset{\sim}{0}) = 0$, no solution in $\mathscr{G}^M$ can escape to infinity. It is to be noted that the equations (18) can be derived from h as a Hamiltonian, if one introduces the Poisson brackets

$$\{\alpha(\underset{\sim}{k}),\ \alpha^*(\underset{\sim}{q})\} = i\,\delta_{\underset{\sim}{k},\underset{\sim}{q}}\ ,\quad \{\alpha(\underset{\sim}{k}),\ \alpha(\underset{\sim}{q})\} = 0\ ,$$

$$\{\alpha(\underset{\sim}{k}),\ \sigma^i(\underset{\sim}{q})\} = 0\qquad ,\quad \{\sigma^+(\underset{\sim}{k}),\ \sigma^-(\underset{\sim}{q})\} = 2i\,\sigma^3(\underset{\sim}{k}+\underset{\sim}{q})\ , \tag{22}$$

$$\{\sigma^3(\underset{\sim}{k}),\ \sigma^\pm(\underset{\sim}{q})\} = \pm\, i\,\sigma^\pm(\underset{\sim}{k}+\underset{\sim}{q})\ .$$

We remark that if N is a cavity with $L(N) = 2^n L(M)$ for some $n \in \mathbb{Z}_+$, then $\Gamma(N) \supset \Gamma(M)$ and the modes in M form a subset of those in N. Similarly, $\mathcal{G}^M$ is a subspace of $\mathcal{G}^N$, which is invariant under the time evolution (18).

Let us fix M and consider a sequence $N \to \infty$ with $\Gamma(N) \supset \Gamma(M)$. Let $H^M_{(N)}$ be the Hamiltonian (12), where one retains in (13) only the coupling between modes in $\Gamma(M)$. Consider the observables

$$\rho_{(N)} = \{\rho^i_{(N)}\} = \{\alpha^\#_{(N)}(\underset{\sim}{k}),\ \sigma^i_{(N)}(\underset{\sim}{k}) \mid \underset{\sim}{k} \in \Gamma(M)\}\ . \tag{23}$$

We shall see that for all t, the operators

$$\rho^i_{(N)}(t) = \exp\,(i\,H^M_{(N)}t)\ \rho^i_{(N)}\ \exp\,(-i\,H^M_{(N)}t)$$

converge in a very weak sense towards the classical solutions $\rho^i(t)$ of (18).

A sequence $\omega_{(N)}$ of density matrices on $\mathcal{H}^A_{(N)} \otimes \mathcal{H}^P_{(N)}$ (i.e., of states of the atoms and of the radiation field in an increasing family of cavities) is called 2-classical (see [3], [4]) with respect to the $\rho_{(N)}$ of the form (23) with value at $\rho \in \mathcal{G}^M$, if

$$\lim_{N\to\infty} \sup_i\ \omega_{(N)}\ \left[(\rho^i_{(N)} - \rho^i)^*\ (\rho^i_{(N)} - \rho^i)\right] = 0 \tag{24}$$

By the Schwarz inequality

$$\lim_{N\to\infty} \omega_{(N)}\ (\rho^i_{(N)}) = \rho^i\ ,$$

$$\lim_{N\to\infty} \omega_{(N)}\ (\rho^i_{(N)}\ \rho^j_{(N)}) = \rho^i\rho^j\ , \tag{25}$$

and hence the observables $\rho_{(N)}$ assume the classical value ρ at least in mean and covariance.

Theorem 1. If $\omega_{(N)}$ is 2-classical for $\rho_{(N)}$ at $\rho \in \mathcal{S}^M$, then $\omega_{(N)}$ is 2-classical for all $\rho_{(N)}(t)$ at $\rho(t)$, the unique solution of (18) with $\rho(0) = \rho$.

Proof: The difference $\rho_{(N)}(t) - \rho(t)$ satisfies a linear differential equation

$$\left(i\omega_k + \frac{d}{dt}\right)\left(\rho^k_{(N)}(t) - \rho^k(t)\right) = \sum_{j=1}^{\infty} A^{kj}_{(N)}(t)\left(\rho^j_{(N)}(t) - \rho^j(t)\right) \tag{26}$$

where the $\omega_k \in \mathbb{R}$ and the $A^{kj}_{(N)}(t)$ are bounded linear operatoars on $\mathcal{H}_{(N)}$ with

$$\sup_{k,N,t} \sum_j \left\| A^{kj}_{(N)}(t) \right\| = A < \infty \,. \tag{27}$$

This follows immediately from the fact that $\lambda(\underset{\sim}{k})$ and $\mu(\underset{\sim}{k})$ are summable and from writing, e.g.,

$$\begin{aligned}
&\left(i\varepsilon + \frac{d}{dt}\right)\left(\sigma^-_{(N)}(\underset{\sim}{k},t) - \sigma^-(\underset{\sim}{k},t)\right) = \\
&= 2i \sum_{\underset{\sim}{q} \in \Gamma(M)} \lambda(\underset{\sim}{q})\, \sigma^3_{(N)}(\underset{\sim}{k}+\underset{\sim}{q},t)\left(\alpha_{(N)}(\underset{\sim}{q},t) - \alpha(\underset{\sim}{q},t)\right) \\
&+ 2i \sum_{\underset{\sim}{q} \in \Gamma(M)} \lambda(\underset{\sim}{q})\, \alpha(\underset{\sim}{q},t)\left[\sigma^3_{(N)}(\underset{\sim}{k}+\underset{\sim}{q},t) - \sigma^3(\underset{\sim}{k}+\underset{\sim}{q},t)\right] \\
&+ \text{similar terms} \,,
\end{aligned} \tag{28}$$

and by observing that $\left\|\sigma^i_{(N)}(\underset{\sim}{q},t)\right\| = 1$. By iteration one obtains the estimate

$$\begin{aligned}
&\sup_i \omega_{(N)}\left[\left(\rho^i_{(N)}(t) - \rho^i(t)\right)^* \left(\rho^i_{(N)}(t) - \rho^i(t)\right)\right] \\
&\leq e^{2A|t|} \sup_i \omega_{(N)}\left[\left(\rho^i_{(N)} - \rho^i\right)^* \left(\rho^i_{(N)} - \rho^i\right)\right] \,.
\end{aligned} \tag{29}$$

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Examples of classical states are "coherent states" (see reference [3]). Let e.g. $\sum_{\underset{\sim}{k} \in \Gamma(M)} |\alpha(\underset{\sim}{k})|^2 < \infty$ and consider the pure state

$$\Omega_{(N)} = \exp\left(\sqrt{N} \sum_{\underset{\sim}{k} \in \Gamma(M)} \{\alpha(\underset{\sim}{k})\, a^*(\underset{\sim}{k}) - \alpha^*(\underset{\sim}{k}) a(\underset{\sim}{k})\}\right) \times \Omega^P \otimes \bigotimes_{n=1}^{N} \left(e^0_{+n} \otimes e^0_{-n}\right) \quad . \tag{30}$$

By (1), (2), (9) and (10) one can verify that $\omega_{(N)} = (\Omega_{(N)}, \cdot \Omega_{(N)})$ is classical at $\{\alpha(\underset{\sim}{k}),\ \sigma^+(\underset{\sim}{k}) = 0,\ \sigma^3(\underset{\sim}{k}) = -\frac{1}{2}\delta_{\underset{\sim}{k},\underset{\sim}{0}}\}$.

Later we shall formulate a much stronger result about the approach to the classical limit.

The classical equations (18) simplify considerably in the rotating wave approximation, if at t = 0 only one mode $\alpha(\underset{\sim}{k}) = \alpha$, $\sigma^+(\underset{\sim}{k}) = \sigma^+ = (\sigma^-)^*$ = $\sigma^-(-\underset{\sim}{k})^*$ and $\sigma^3(\underset{\sim}{0}) = \sigma^3$ is excited. It is easily seen that this state of affairs will persist for all times, and we obtain the classical one-mode laser equations (in the rotating wave approximation and without reservoirs):

$$\begin{aligned} \dot{\alpha} &= -i\nu\alpha - i\lambda\sigma^- \\ \dot{\sigma}^- &= -i\varepsilon\sigma^- + 2i\lambda\sigma^3\alpha \\ \dot{\sigma} &= i\lambda(\sigma^-\alpha^* - \sigma^+\alpha) \end{aligned} \tag{31}$$

Besides h and s, (31) has the integral $c = |\alpha|^2 + \sigma^3$ (see (14)) and $\{h,s\} = \{h,c\} = \{s,c\} = 0$. It can be shown that (31) is an integrable system with invariant tori. The allowed physical values of s are $0 \leq s \leq 1/4$.

Simple special solutions of (31) are

(a) Trivial stationary solutions

$$-\frac{1}{2} \leq \sigma^3 = \text{const.} \leq \frac{1}{2}\ , \quad \sigma^+ = \alpha = 0\ . \tag{32}$$

(b) Nontrivial stationary solutions

$$\sigma^3 = -\frac{\varepsilon\nu}{2\lambda^2}\ , \quad \alpha = -\lambda\sigma^-/\nu = \text{const.}\ , \tag{33}$$

which are physically admissible only for large coupling constants, for $\varepsilon\nu \leq \lambda^2$.

(c) Harmonic solutions $\sigma^-(t) = e^{-i\omega t}\sigma^-$, $\alpha(t) = e^{-i\omega t}\alpha$,

$$\sigma^- = \frac{\omega-\nu}{\lambda}\,\alpha = \text{const.}\ , \quad \sigma^3 = -\,(\varepsilon-\omega)\,(\nu-\omega)/2\lambda^2\ . \tag{34}$$

The stationary solutions (32) and (33) are particularly important for equilibrium statistical mechanics: the Gibbs state at the reciprocal temperature β is of the form (33) averaged over $\arg\alpha$, if β is large enough and if $\varepsilon\nu < \lambda^2$. If β is small, then the Gibbs state is of the form (32). Thus, if $\varepsilon\nu < \lambda^2$, a phase transition occurs from a state in which the expected photon number is of O(N), to a state in which it is O(1).

The critical value of β for the equilibrium phase transition is

$$\beta_c = \frac{2}{\varepsilon}\,\tanh^{-1}\left(\frac{\nu\varepsilon}{\lambda^2}\right)\ . \tag{35}$$

We shall not discuss here the thermodynamics of the laser, which can be found in [5], [6], [7].

5. THE ATOMIC RESERVOIRS

The physical picture which we have in mind of the atomic dissipation and pumping is a coupling of the localized electron states of each atom to the surrounding electrons which has the property of draining or filling the two atomic energy levels. We shall do this in such a way that the mean electron number of each atom is one, and will remain so for all time. While there are fluctuations in the individual atomic electron numbers of order one, the total number fluctuations will be only of order $N^{1/2}$. This fact will be demonstrated later.

Consider the nth atom, $1 \leq n \leq N$, with creation and annihilation operators $b^{\#}_{+n}$ and $b^{\#}_{-n}$. We shall drop the label n until it becomes necessary. The reservoir for this atom consists of four fermion fields labelled by the continuous parameter $w \in \mathbb{R}$ with creation and annihilation operators $B^{\#}_{\pm}(w)$, $C^{\#}_{\pm}(w)$. The reservoir Hamiltonian is $H^{AR} = H^{AR}_0 + H^{AR}_1$,

$$H^{AR}_0 = \sum_{\pm}\int_{-\infty}^{+\infty} dw\ w\,[B^*_{\pm}(w)\ B_{\pm}(w) + C^*_{\pm}(w)\ C_{\pm}(w)] \tag{36}$$

$$H^{AR}_1 = \sum_{\pm}\int_{-\infty}^{+\infty} dw\ [g^B_{\pm}(w)\ B^*_{\pm}(w) b_{\pm} + g^C_{\pm}(w)\ C^*_{\pm}(w) b^*_{\pm} + \text{h.c.}]\ ,$$

where $g^B_{\pm}$, $g^C_{\pm}$ are real functions to be specified later.

These fermion fields anticommute with the $b_\pm$ operators of the same index $\pm$ and commute with all operators of a different index. For the same index, the anticommutators, $\{A,B\} = AB + BA$, are

$$\{B^*(w),\ B(w')\} = \delta(w-w') = \{C^*(w),\ C(w')\}\ , \qquad (37)$$

$$\{b^*, b\} = 1$$

and all other anticommutators between such $B^\#$, $C^\#$, $b^\#$ are zero. It is important to note that H_0^{AR} is self-adjoint in the Fock representation, where

$$B_\pm(w)\ \Omega^{AR} = C_\pm(w)\ \Omega^{AR} = 0 \qquad (38)$$

for all w. If $g_\pm^B,\ g_\pm^C \in L^2$, then H_1^{AR} is bounded.

The Heisenberg equations of motion of the $B^\#$ and $C^\#$ operators are

$$\begin{aligned} \dot{B}_\pm(w,t) &= -iw\ B_\pm(w,t) - ig_\pm^B(w)\ b(t) \\ \dot{C}_\pm^*(w,t) &= \ \ iw\ C_\pm^*(w,t) + ig_\pm^C(w)\ b(t) \end{aligned} \qquad (39)$$

Thus

$$B_\pm(w,t) = e^{-iwt}\ B_\pm(w) - ig_\pm^B(w) \int_0^t ds\ e^{-iw(t-s)}\ b_\pm(s) \qquad (40)$$

and similarly for $C_\pm(w,t)$.

The Heisenberg equations of motion for the $b_\pm$-operators are

$$\begin{aligned} \dot{b}_\pm(t) &= i[H^A + H^{AP} + H^{AR}\ ,\ b_\pm(t)] \\ &= i[H^A + H^{AP},\ b_\pm(t)] \\ &\quad - i \int_{-\infty}^{+\infty} dw\ [g_\pm^B(w)\ B(w,t) - g_\pm^C(w)\ C_\pm^*(w,t)]\ . \end{aligned} \qquad (41)$$

The expressions for $B_\pm$ and $C_\pm$ obtained above can be inserted into (41). In this section we primarily wish to study the effects of the reservoir on the $b_\pm$-operators, and to that end shall temporarily drop the terms involving H^A and H^{AP}. Equation (41) then becomes

$$\dot{b}_{\pm}(t) = -\int_0^t ds\, b_{\pm}(s) \int_{-\infty}^{+\infty} dw \left(g_{\pm}^{B}(w)^2\, e^{-iw(t-s)} + g_{\pm}^{C}(w)^2\, e^{iw(t-s)}\right) \tag{42}$$

$$- i \int_{-\infty}^{+\infty} dw \left(g_{\pm}^{B}(w)\, e^{-iwt}\, B_{\pm}(w) - g_{\pm}^{C}(w)\, e^{iwt}\, C_{\pm}^{*}(w)\right) .$$

The second term is a definite time-dependent operator, $f_{\pm}(t)$, which depends only on the observables of the reservoir at time zero, and which we shall call a "fluctuation force". To make further progress we shall assume that

$$g_{\pm}^{B,C}(w) = g_{\pm}^{B,C}\, \tau(w^2 + \tau^2)^{-1/2} \tag{43}$$

with $g_{\pm}^{B,C} \geq 0$, $\tau > 0$. Then with $\gamma_{\pm} = \pi((g_{\pm}^{B})^2 + (g_{\pm}^{C})^2)$ equation (42) becomes

$$\dot{b}_{\pm}(t) = -\gamma_{\pm}\tau \int_0^t ds\, e^{-\tau(t-s)}\, b_{\pm}(s) + f_{\pm}(t) . \tag{44}$$

The first term is a damping term with memory. For our Lorentzian cutoff, (44) is a second order linear inhomogeneous differential equation

$$\ddot{b}_{\pm}(t) = -\gamma_{\pm}\tau\, b_{\pm}(t) - \tau\, \dot{b}_{\pm}(t) + \dot{f}_{\pm}(t) + \tau f_{\pm}(t) \tag{45}$$

with initial conditions

$$\begin{aligned} b_{\pm}(0) &= b_{\pm} , \\ \dot{b}_{\pm}(0) &= f_{\pm}(0) . \end{aligned} \tag{46}$$

For large τ, the solutions to the homogeneous equation decay as $e^{-\tau t}$ and $e^{-\gamma_{\pm} t}$.

In the spirit of dynamical systems, we have to specify the initial state of the fermion and its reservoir in order to determine the expectation values of the observables at all later times. Mathematically, the assumptions that at time $t = 0$ one puts together the system and reservoir in an uncorrelated way means that the initial state ω is a tensor product, $\omega = \omega^S \otimes \omega^R$, of a state of the system, ω^S, and of the reservoir, ω^R. A state ω^R of a quantum system of infinitely many degrees of freedom with an algebra of observables, $\mathcal{U}^R$, generated by all polynomials in $B_{\pm}^{\#}(w)$, $C_{\pm}^{\#}(w)$ (smeared out over L^2 test functions in w) is a positive normalized linear functional on $\mathcal{U}^R$ [8]. We may assume that at $t = 0$ the reservoir is in thermal equilibrium, and hence in the Gibbs state for the H_0^{AR}-time evolution of $\mathcal{U}^R$. However, in order to avoid technical complications we shall restrict ourselves to the Fock state (38).

The atom, when coupled to this reservoir, shows an exponential approach to equilibrium. If ω^S is any density matrix on $\mathcal{V}$, then as $t \to +\infty$,

$$\omega^S \otimes \omega^R (b_\pm^\#(t)) \to 0$$

$$\omega^S \otimes \omega^R (b_\pm^\#(t)\, b_\mp^\#(t)) \to 0 \qquad (47)$$

and

$$\omega^S \otimes \omega^R (b_\pm^*(t)\, b_\pm(t)) \to I_\pm \ . \qquad (48)$$

The algebraic computations simplify greatly if one takes the limit $\tau \to \infty$, $g_\pm^{B,C}(w) \to g_\pm^{B,C}$, in which case the time evolution continues to make sense as a 1-parameter group of automorphisms of $\mathcal{U} = \mathcal{U}^S \otimes \mathcal{U}^R$, where $\mathcal{U}^S$ are the bounded operators on $\mathcal{H}^S$:

$$\dot{b}_\pm(t) = -\gamma_\pm b_\pm(t) + f_\pm(t)$$

$$b_\pm(t) = e^{-\gamma_\pm t} b_\pm + \int_0^t ds\, e^{-\gamma_\pm(t-s)} f_\pm(s) \ , \qquad (49)$$

and in this case,

$$I_\pm = (g_\pm^C)^2 \left[(g_\pm^B)^2 + (g_\pm^C)^2\right]^{-1} \ . \qquad (50)$$

As one sees from (48) the quantities $I_\pm$ are the $t \to \infty$ limit of the occupations in the upper and lower atomic levels. These quantities are determined by the parameters of the reservoir, namely $(g_\pm^B)^2$ and $(g_\pm^C)^2$. We wish to adjust them so that three conditions are satisfied:

(i) The asymptotic electron number is unity. This requires that

$$I_+ + I_- = 1 \qquad (51)$$

(ii) The asymptotic "atomic inversion", namely the average difference between the number of electrons in the upper level and in the lower level, is some specified number η. This requires that

$$\frac{1}{2}(I_+ - I_-) = \eta \qquad (52)$$

(iii) The third condition is one whose significance will only become apparent later when we couple the atoms to the radiation field. As a consequence of (38) and (44), the equations of motion for $N_\pm \equiv \omega^S \otimes \omega^R \left(b_\pm^*(t)\, b_\pm(t)\right)$ are

$$\dot{N}_{\pm}(t) = -2\gamma_{\pm}(N_{\pm}(t) - I_{\pm}) \tag{53}$$

The equations of quantum electrodynamics (15) only involve the operators $S^1(\underset{\sim}{k})$. By definition, the expectation value of S^3 is $\frac{1}{2}(N_+ - N_-)$. Owing to the interaction with the radiation field, $N_+ - N_-$ may not approach the value $I_+ - I_-$ for $t \to +\infty$, which as we demonstrated happens for an isolated atom. By (53) this would force $N_+ + N_-$ to approach a value other than 1, unless we set

$$\gamma_+ = \gamma_- = \gamma/2 \ . \tag{54}$$

This choice also has the important advantage that for the isolated atom $N_+ + N_- = 1$ for all times if $N_+ + N_- = 1$ at $t = 0$.

An elementary computation shows that one has to choose

$$(g_+^B)^2 = (g_-^C)^2 \quad , \quad (g_+^C)^2 = (g_-^B)^2 \ . \tag{55}$$

There remain two free parameters:

$$\begin{aligned} \gamma &= 2\pi\left((g_+^B)^2 + (g_-^B)^2\right) \ , \\ \eta &= \left((g_-^B)^2 - (g_+^B)^2\right)/2\left((g_+^B)^2 + (g_-^B)^2\right) \ , \end{aligned} \tag{56}$$

and the whole region $-1/2 \leq \eta \leq 1/2$ can be reached.

The results of this section can be summarized as follows: Each electron state of each atom is driven by its reservoir in such a way that the mean electron number per atom approaches unity, if it was not at that value initially, the mean value of S^3 is pumped to the value η, and the mean value of $S^{\pm}$ goes to zero.

6. THE PHOTON RESERVOIRS

Similarly to the atom-reservoir system, we introduce a photon reservoir which will have the effect of damping the photon modes. This photon damping is necessary; otherwise the equations of motion we shall subsequently develop will have no bounded stationary states for $\eta > 0$. Damping occurs, of course, in a real laser in the form of losses at the cavity walls and mirrors.

As a mathematical model of a photon reservoir we take a separate reservoir for each photon mode designated by the wave vector $\underset{\sim}{k}$. This reservoir has boson creation and annihilation operators $A^{\#}(\underset{\sim}{k},w)$ with commutation relations

$$[A(\underset{\sim}{k},w),\ A^*(\underset{\sim}{k}',w')] = \delta_{\underset{\sim}{k},\underset{\sim}{k}'}\ \delta(w-w') \tag{57}$$

and all other commutators vanish. In the above, the first δ is a Kronecker delta and the second δ is a Dirac delta function. The Hamiltonian for these reservoirs is

$$H^{PR} = \sum_{\underset{\sim}{k}} \int_{-\infty}^{+\infty} dw \left\{ w\, A^*(\underset{\sim}{k},w)\, A(\underset{\sim}{k},w) + \tau\, h(\underset{\sim}{k})\, (w^2+\tau^2)^{-1/2} \left[A^*(\underset{\sim}{k},w)\, a(\underset{\sim}{k}) + a^*(\underset{\sim}{k})\, A(\underset{\sim}{k},w)\right]\right\} \tag{58}$$

In this section we shall suppress the index $\underset{\sim}{k}$. The equations of motion for a photon coupled to its reservoir can be derived as in Section 5. In the absence of a coupling to the atoms, the solution is the integro-differential equation

$$\dot{a}(t) = -\tau\kappa \int_0^t ds\, e^{-\tau(t-s)}\, a(s) - ih \int_{-\infty}^{+\infty} \frac{\tau\, dw}{(w^2+\tau^2)^{1/2}}\, A(w)\, e^{-iwt} \tag{59}$$

with $\kappa = \pi h^2$. The solution of (59) is similar to the one of (45). In the limit $\tau \to \infty$ we obtain

$$a(t) = e^{-\kappa t}\, a + \int_0^t ds\, e^{-\kappa(t-s)}\, f(s) \tag{60}$$

where $f(s) = -ih \int dw\, A(w)\, e^{-iwt}$ is again a fluctuation force.

As the state of the reservoir we take a pure state, the Fock vacuum Ω^{PR} which satisfies for all w

$$A(w)\, \Omega^{PR} = 0 \ . \tag{61}$$

Then, for an arbitrary state ω^S of the photon, for which $\omega^S(a^*a) < \infty$ at t=0, one has

$$\lim_{t\to\infty} \omega^S \otimes \omega^R \left(a^*(t)\, a(t)\right) = 0 \ . \tag{62}$$

In [4] we took another model for the photons and their reservoirs. There we built the photons out of infinitely many fermions, each of which had a fermion field as reservoir. Then the construction of Section 5 is applicable, including finite temperature Gibbs states for the reservoirs.

7. THE FULLY COUPLED LASER

In order to gain an understanding of the cooperative properties of the full laser-reservoir system, we shall first describe the one mode laser in the rotating wave approximation. Now the Hamiltonian is

$$H_{(N)} = H^{P}_{(N)} + H^{A}_{(N)} + H^{AP}_{(N)} + H^{AR}_{(N)} + H^{PR}_{(N)} \ . \tag{63}$$

The first three terms together are the Hamiltonian of the laser proper (with restriction to the modes of a fixed large cavity M). The last two terms are the reservoir Hamiltonians; these are the Hamiltonians described in equations (36) and (58) summed over all the atoms. Again, to simplify matters, we shall first take the singular reservoirs, by passing to the limits $\tau \to \infty$ in all reservoirs.

As before we are interested in the intensive observables

$$\sigma^{i}_{(N)} = N^{-1} S^{i}_{(N)} \text{ and } \alpha_{(N)} = N^{-1/2} a, \ i \in \{+,-,3\}.$$

The Heisenberg equations of motion are

$$\begin{aligned}
\dot{\alpha}_{(N)}(t) &= -(\kappa+i\nu)\ \alpha_{(N)}(t) - i\lambda\ \sigma^{-}_{(N)}(t) + \Phi_{(N)}(t) \\
\dot{\sigma}^{-}_{(N)}(t) &= -(\gamma+i\varepsilon)\ \sigma^{-}_{(N)}(t) + 2i\lambda\ \sigma^{3}_{(N)}(t)\ \alpha_{(N)}(t) + \chi^{-}_{(N)}(t) \\
\dot{\sigma}^{3}_{(N)}(t) &= -\gamma(\sigma^{3}_{(N)}(t)-\eta) + i\lambda[\sigma^{-}_{(N)}(t)\ \alpha^{*}_{(N)}(t) - \sigma^{+}_{(N)}(t)\ \alpha_{(N)}(t)] \\
&\quad + \chi^{3}_{(N)}(t) \ .
\end{aligned} \tag{64}$$

The influence of the photon reservoir shows up in two ways: in a systematic damping term, $-\kappa\ \alpha_{(N)}(t)$, which depends only on the state of the small system and which is hopefully O(1) as $N \to \infty$, and in a fluctuation force

$$\Phi_{(N)}(t) = -ih \int_{-\infty}^{+\infty} dw\ e^{-iwt}\ A(w)\ /\ \sqrt{N} \tag{65}$$

which is manifestly $O(N^{-1/2})$ and which only depends on the initial state of the reservoir. In the equations for the atomic observables the damping terms, $-\ \gamma\ \sigma^{i}_{(N)}(t)$, arise from contributions from all electrons according to (49). The fluctuation forces $\chi^{i}_{(N)}(t)$ come from the second term on the right side of (49), and they are very complicated for finite N:

$$\chi^{-}_{(N)}(t) = N^{-1} \sum_{n=1}^{N} \left\{ b^{*}_{-n}(t)\ f_{+n}(t) + f^{*}_{-n}(t)\ b_{+n}(t) \right\} \ , \tag{66}$$

where, according to (42),

$$f_{\pm n}(t) = -i \int_{-\infty}^{+\infty} dw \, [g_{\pm}^{B} B_{\pm n}(w) \, e^{-iwt} - g_{\pm}^{C} C_{\pm n}^{*}(w) \, e^{iwt}] \tag{67}$$

and

$$\chi_{(N)}^{3}(t) = (2N)^{-1} \sum_{n=1}^{N} \{ b_{+n}^{*}(t) \, f_{+n}(t) + f_{+n}^{*}(t) \, b_{+n}(t) - b_{-n}^{*}(t) \, f_{-n}(t) - f_{-n}^{*}(t) \, b_{-n}(t) \} - \gamma\eta \tag{68}$$

The constant $\gamma\eta$ has been subtracted on the right side of (68) in order that for $i \in \{+,-,3\}$ and all t

$$\omega^{R}(\chi_{(N)}^{i}(t)) = 0 \, . \tag{69}$$

We have previously computed η to be (56) for noninteracting atoms. It can be shown from the anticommutation relations of the $b^{\#}$'s, which are preserved in time, and from (38) and (49) that (69) holds with the same value of η for all times.

If the atoms were uncoupled, then the $\chi_{(N)}^{i}$ would each be a sum of identically distributed independent random variables with mean zero. By the law of large numbers the $\chi_{(N)}^{i}$ would be $O(N^{-1/2})$ for $N \to \infty$. In our model, the $b_{\pm n}^{\#}(t)$ are weakly dependent on each other, through the radiation field, but it is a theorem (see References [4], [5] and Theorem 2 below) that for a suitable choice of classical states the $\chi_{(N)}^{i}$ can be neglected in the equations (64) as $N \to \infty$. Furthermore, the $\alpha_{(N)}(t)$ and $\sigma_{(N)}^{i}(t)$ converge, as they did in Theorem 1, to complex solutions of the classical laser equations

$$\begin{aligned} \dot{\alpha}(t) &= -(\kappa+i\nu)\,\alpha(t) - i\lambda\,\sigma^{-}(t) \\ \dot{\sigma}^{-}(t) &= -(\gamma+i\varepsilon)\,\sigma^{-}(t) + 2i\lambda\,\sigma^{3}(t)\,\alpha(t) \\ \dot{\sigma}^{3}(t) &= -\gamma(\sigma^{3}(t)-\eta) + i\lambda(\sigma^{-}(t)\,\alpha^{*}(t) - \sigma^{+}(t)\,\alpha(t)) \end{aligned} \tag{70}$$

with initial value $\alpha(0) = \alpha$, $\sigma^{i}(0) = \sigma^{i}$ determined by the state ω^{S}.

There is one additional intensive observable of the atoms to which we should pay attention, the mean number of electrons

$$\nu_{(N)}(t) = N^{-1} \sum_{n=1}^{N} \{ b_{+n}^{*}(t) \, b_{+n}(t) + b_{-n}^{*}(t) \, b_{-n}(t) \} \, . \tag{71}$$

In the fully coupled laser (63), $\nu_{(N)}(t)$ satisfies

$$\dot{\nu}_{(N)}(t) = -\gamma(\nu_{(N)}(t)-1) + \psi_{(N)}(t) \ . \tag{72}$$

The term $(-\gamma)(-1)$ is a result of (55). The $\psi_{(N)}(t)$ is a fluctuation force of the type given before. If one believes the previous argument that fluctuation forces can be neglected on the macroscopic level as $N \to \infty$, one sees that the dissipation maintains the mean electron number at unity.

Next we shall describe the properties of these classical equations. There is a Liapunov function

$$L(t) = |\alpha(t)|^2 + \sigma^3(t) + |\sigma^-(t)|^2 + |\sigma^3(t)|^2 \ , \tag{73}$$

which is bounded from below and satisfies

$$\dot{L}(t) < 0 \text{ for } |\alpha(t)|^2 + |\sigma^+(t)|^2 + |\sigma^3(t)|^2$$

outside of some sphere in the 5-dimensional phase space. Hence all solutions of (70) stay bounded for all times.

The only stationary solution is

$$\sigma^3 = \eta \ , \ \sigma^- = \alpha = 0 \ . \tag{74}$$

This solution is asymptotically stable for

$$\eta < \eta^C = \frac{\kappa\gamma}{2\lambda^2}\left(1 + \frac{(\varepsilon-\nu)^2}{(\kappa+\gamma)^2}\right) \tag{75}$$

If η passes the threshold η^C, a Hopf bifurcation occurs and a one-parameter family of periodic solutions becomes attracting:

$$\begin{aligned} &\alpha(t) = \alpha\, e^{-i\omega t} \ , \quad \sigma^-(t) = \sigma^-\, e^{-i\omega t} \ , \\ &\sigma^3(t) = \eta^C \ , \quad \omega = \frac{\kappa\varepsilon + \gamma\nu}{\kappa + \gamma} \ , \\ &(\kappa+i(\nu-\omega))\alpha = -i\lambda\sigma^- \ , \quad |\alpha|^2 = \frac{\gamma}{2\kappa}(\eta-\eta^C) \ . \end{aligned} \tag{76}$$

It is possible that there are further bifurcations and, indeed, for the multimode laser one can exhibit such phenomena.

The physical interpretation of η^C is that it is the critical pumping constant for a reservoir-driven phase transition from a non-radiating to a coherently radiating oscillatory state. In the non-vanishing stationary state the atoms and photons behave as though they are uncoupled and influenced only by their reservoirs. The oscillatory state is truly cooperative and has a frequency ω which is a convex combination of the cavity and atomic frequencies.

There is an obvious generalization of (70) to the case of infinitely many modes $\underset{\sim}{k} \in \Gamma(M)$ associated with a cavity of fixed length $L(M)$ and without making the rotating wave approximation. It is clear that there again exists a transition from a stationary to a radiating state. However, the detailed description of the bifurcations becomes truly complicated.

Another level of complication arises if one takes regular reservoirs for the atoms. We have derived only the equations for the Lorentzian cut-off $g(w) = g\tau(w^2+\tau^2)^{-1/2}$. By (45) the photon and atomic observables satisfy second order differential equations in this case. Hence more intensive observables are necessary to describe the macroscopic behavior of the atoms. In addition to the $\sigma^i_{(N)}$ and $\alpha_{(N)}$ they are

$$\begin{aligned}
\sigma^{+'}_{(N)}(t) &= N^{-1} \sum_{n=1}^{N} \dot{b}^*_{+n}(t)\, \dot{b}_{-n}(t) = \sigma^{-'}_{(N)}(t)^* \\
\sigma^{3'}_{(N)}(t) &= (2N)^{-1} \sum_{n=1}^{N} \left(b^*_{+n}(t)\, \dot{b}_{+n}(t) - \dot{b}^*_{-n}(t)\, b_{-n}(t)\right) \\
&= \sigma^{3''}_{(N)}(t)^* \\
\sigma^{3'''}_{(N)}(t) &= (2N)^{-1} \sum_{n=1}^{N} \left(\dot{b}^*_{+n}(t)\, \dot{b}_{+n}(t) - \dot{b}^*_{-n}(t)\, \dot{b}_{-n}(t)\right)
\end{aligned} \tag{77}$$

In the rotating wave approximation and for maximal pumping, $\eta = \frac{1}{2}$, the classical laser equations become (for $N \to \infty$):

$$\begin{aligned}
\ddot{\sigma}^+ &= -\tau(\gamma - i\varepsilon)\sigma^+ + \left(\frac{i\varepsilon}{2} - \tau\right)\dot{\sigma}^+ + 2\sigma^{+'} \\
&\quad - 2i\lambda\tau\alpha^*\sigma^3 - 2i\lambda\dot{\alpha}^*\sigma^3 - 2i\lambda\alpha^*\sigma^{3'} \\
\dot{\sigma}^{+'} &= \frac{\tau}{2}(i\varepsilon - \gamma)\dot{\sigma}^+ + (i\varepsilon - 2\tau)\sigma^{+'} - 2i\lambda(\dot{\alpha}^* + \tau\alpha^*)\sigma^{3''} - 2i\lambda\alpha^*\sigma^{3'''} \\
\dot{\sigma}^3 &= \sigma^{3'} + \sigma^{3''} \\
\dot{\sigma}^{3'} &= -\frac{\tau}{2}(i\varepsilon + \gamma)\sigma^3 - \left(\tau + \frac{i\varepsilon}{2}\right)\sigma^{3'} + \sigma^{3'''} \\
&\quad - i\lambda\dot{\alpha}\sigma^+ - \frac{i\lambda}{2}\alpha\dot{\sigma}^+ - i\lambda\tau\alpha\sigma^+ \\
\dot{\sigma}^{3'''} &= -\frac{\tau}{2}(\gamma - i\varepsilon)\sigma^{3'} - \frac{\tau}{2}(\gamma + i\varepsilon)\sigma^{3''} - 2\tau\sigma^{3'''} \\
&\quad - i\lambda\alpha\sigma^{+'} + i\lambda\alpha^*\sigma^{-'} - \frac{i\lambda}{2}\dot{\alpha}\dot{\sigma}^+ + \frac{i\lambda}{2}\dot{\alpha}^*\dot{\sigma}^- + \frac{\gamma\tau^2}{2} \\
\ddot{\alpha} &= -(\tau + i\nu)\dot{\alpha} - \tau(i\nu + \kappa)\alpha - i\lambda\dot{\sigma}^- - i\lambda\tau\sigma^- .
\end{aligned} \tag{78}$$

One sees by inspection that these equations have a stationary solution, where the only nonvanishing amplitudes are

$$\sigma^3 = \frac{1}{2} \ , \ \sigma^{3'} = -\frac{i\varepsilon}{4} \ , \ \sigma^{3'''} = \frac{\gamma\tau}{4} + \frac{\varepsilon^2}{8} \ . \tag{79}$$

This solution is stable for small coupling $|\lambda|$. For $\varepsilon = \nu = 0$, $\eta = 1/2$ and τ sufficiently large, (79) becomes unstable for $\lambda^2 = \lambda_c^2 = \kappa\gamma$, just as in (75). For large τ and $\varepsilon > 0$ and $\nu > 0$ the constant term in the characteristic polynomial for (78) linearized around (79) does not vanish. Hence, the unstable attractor bifurcates into a stable periodic solution, and the qualitative behavior of the one-mode laser remains unchanged for these more complicated but physically more realistic reservoirs.

What we have said so far, without proof, is that the quantities

$$\lim_{N\to\infty} \omega_{(N)}(\sigma^i_{(N)}(t))$$

satisfy the classical equations of motion given above when the sequence of states $\omega_{(N)}$ is classical. We now wish to investigate the next lower order in $N^{1/2}$, namely expectations of the algebra generated by the fluctuation observables

$$a_{(N)}(t) = N^{1/2}\,[\alpha_{(N)}(t)-\alpha(t)] \text{ and } s^i_{(N)}(t) = N^{1/2}[\sigma^i_{(N)}(t) - \sigma^i(t)] .$$

Clearly the fluctuation forces which have heretofore been neglected will now play a decisive role. The equal time commutators between fluctuation observables are intensive observables, e.g.,

$$\begin{aligned} [a_{(N)}(t),\ a^*_{(N)}(t)] &= 1 \\ [s^+_{(N)}(t),\ s^-_{(N)}(t)] &= 2\sigma^3_{(N)}(t) . \end{aligned} \tag{80}$$

Hence in the limit $N \to \infty$ they should become numbers.

One would hope that equations of motion for the $a_{(N)}(t)$ and $s^i_{(N)}(t)$ could be obtained as follows: Take the full equations of motion, including the fluctuation forces, and linearize them around the classical orbits which are regarded as having been determined given the initial expectation value for the intensive observables in $\omega_{(N)}$. In this way one obtains linear equations for the operators $a_{(N)}(t)$ and $s^i_{(N)}(t)$ which have time dependent coefficients given by the numerical functions $\alpha(t)$ and $\sigma^i(t)$ and operator valued inhomogeneous terms $F_{(N)}(t) = \sqrt{N}\,\Phi_{(N)}(t)$, and $G^i_{(N)}(t) = \sqrt{N}\,\chi^i_{(N)}(t)$. Then, in some weak sense for large N, and for the one-mode laser in the rotating wave approximation,

$$\begin{aligned} \dot{a}_{(N)}(t) &= -(\kappa+i\nu)a_{(N)}(t) - i\lambda\, s^-_{(N)}(t) + F_{(N)}(t) \ , \\ \dot{s}^-_{(N)}(t) &= -(\gamma+i\varepsilon)s^-_{(N)}(t) - 2i\lambda\,\alpha(t)\, s^3_{(N)}(t) \\ &\quad + 2i\lambda\,\sigma^3(t)\, a_{(N)}(t) + G^-_{(N)}(t) \ , \end{aligned} \tag{81}$$

$$\dot{s}^3_{(N)}(t) = -\gamma\, s^3_{(N)}(t) + i\lambda\, [\alpha^*(t)\, s^-_{(N)}(t) + \sigma^-(t)\, a^*_{(N)}(t) - \alpha(t)\, s^+_{(N)}(t) - \sigma^+(t)\, a_{(N)}(t)] + G^3_{(N)}(t)$$

We have taken the one-mode laser with rotating wave approximation as an illustrative example, but similar equations could be derived in the other cases.

The meaning of (81) is clear. One solves these linear equations in terms of the initial conditions for the $a_{(N)}(t)$ and $s^i_{(N)}(t)$ and using the $F_{(N)}(t)$, $G^i_{(N)}(t)$ for all t. Assuming that the states are such that the $N \to \infty$ limits of $a_{(N)}(0)$, $s^i_{(N)}(0)$, $F_{(N)}(t)$ and $G^i_{(N)}(t)$ for all t exist, we could calculate the fluctuations and their moments for all t. Note that the same reasoning would apply to the mean electron number and ensures that the fluctuations in the mean electron number are $O(N^{-1/2})$.

If the foregoing reasoning can be justified--and we can in fact do so--the expectation values of the fluctuations of the $a_{(N)}(t)$ and $s^i_{(N)}(t)$ can be computed in terms of the expectation values of the fluctuations $F_{(N)}(t)$ and $G^i_{(N)}(t)$. These in turn require knowledge of the $b_{\pm n}(t)$. It turns out again that the obvious simplification for $N \to \infty$ can be shown to be correct. That is that one returns to the elementary Heisenberg equations of motion for the $b_{\pm n}(t)$ and decouples them by replacing the operator valued function $\alpha_{(N)}(t)$ by the classical function $\alpha(t)$. The terms coming from the time zero reservoir operators are retained, of course. Call this approximate solution $\hat{b}_{\pm n}(t)$ and use it to compute approximate fluctuation forces $\hat{G}^i_{(N)}(t)$ in (66) and (68). The expectation values of these fluctuation forces can easily be calculated (see [3], Chapter 3) and shown to be Gaussian and δ-correlated in time as $N \to \infty$. The relevant fact is that as $N \to \infty$ this simple calculation becomes exact, for

$$\lim_{N\to\infty} (G^i_{(N)}(t) - \hat{G}^i_{(N)}(t)) = 0$$

in a suitable topology described below.

In the above heuristic discussion we have outlined in principle a method of calculating the fluctuations around the classical orbit. The theorem that justifies this will now be given without proof. This latter can be found in references [3] and [4].

Let $\rho_{(N)} = \{\rho^i_{(N)}\}$ be the sequence of intensive observables of the laser model under consideration, namely (23) for the ∞-mode case and $\rho_{(N)} = \{\alpha^\#_{(N)}, \sigma^i_{(N)}, \nu_{(N)}\}$ for the 1-mode laser. Let $\mathcal{G}$ be the phase space of the model. $\mathcal{G}$ is the Hilbert space $\mathcal{G}^M \times \mathbb{R}^1$, if one takes all modes in $\Gamma(M)$ and $\mathcal{G} = \mathbb{R}^6$ for the 1-mode laser. A sequence of density matrices $\omega^S_{(N)}$ on $\mathcal{H}^S_{(N)} = \mathcal{H}^A_{(N)} \otimes \mathcal{H}^P_{(N)}$ is called <u>classical</u> at $\rho \in \mathcal{G}$, if for all monomials of elements in $\rho_{(N)}$

$$\lim_{N\to\infty} \omega^S_{(N)} (\rho^{i_1}_{(N)} \cdots \rho^{i_n}_{(N)}) = \rho^{i_1} \cdots \rho^{i_n} . \qquad (82)$$

In reference [4] such a sequence of states was called pure classical and convex combinations of pure classical states were called classical.

A sequence $\omega^S_{(N)}$ has normal fluctuations around ρ, if for all monomials

$$\lim_{N\to\infty} \omega^S_{(N)} \left(\sqrt{N}\,(\rho^{i_1}_{(N)} - \rho^{i_1}) \ \ldots\ \sqrt{N}\,(\rho^{i_n}_{(N)} - \rho^{i_n})\right) \tag{83}$$

exists. Clearly, a state with normal fluctuations around ρ is classical at ρ, by the Schwarz inequality.

Let $\omega^R_{(N)}$ be a state of the reservoir of the type mentioned in Sections 5 and 6.

Theorem 2. Let $\omega^S_{(N)}$ be classical at $\rho \in \mathcal{G}$. Let $\rho_{(N)}(t)$ be the solution of the Heisenberg equations for the fully coupled laser and let $\rho(t)$ be the solutions of the corresponding classical equations with $\rho(0) = \rho$. Then for all monomials and all times $t_1, \ldots, t_n$

$$\lim_{N\to\infty} \omega^S_{(N)} \otimes \omega^R_{(N)} \left(\rho^{i_1}_{(N)}(t_1) \ \ldots\ \rho^{i_n}_{(N)}(t_n)\right) = \rho^{i_1}(t_1) \ \ldots\ \rho^{i_n}(t_n) \tag{84}$$

uniformly over bounded time intervals.

Theorem 3. Let $\omega^S_{(N)}$ have normal fluctuations around ρ. Let

$$r^i_{(N)}(t) = \sqrt{N}\,\left(\rho^i_{(N)}(t) - \rho^i(t)\right).$$

Let $\hat{r}_{(N)}(t)$ be the solution of the linearized Heisenberg equations of motion as described above with the fluctuation forces for the photons given explicitly, and with the fluctuation forces for the atomic observables calculated by the decoupling scheme mentioned above for the $\hat{b}_{\pm n}(t)$. Then for all times

$$\lim_{N\to\infty} \omega^S_{(N)} \otimes \omega^R_{(N)} \left(r^{i_1}_{(N)}(t_1) \ \ldots\ r^{i_n}_{(N)}(t_n)\right) \tag{85}$$

exists and is equal to

$$\lim_{N\to\infty} \omega^S_{(N)} \otimes \omega^R_{(N)} \left(\hat{r}^{i_1}_{(N)}(t_1) \ \ldots\ \hat{r}^{i_n}_{(N)}(t_n)\right) . \tag{86}$$

This latter limit exists by explicit computation. The limit is uniform on bounded time intervals.

In reference [4] these theorems were proved for a modified dynamics in which the photon operators were replaced by truncated operators having norms $\leq \zeta N$ and behaving as real photons for photon numbers $\ll \zeta N$. In the limit $N \to \infty$ followed by $\zeta \to \infty$ we obtained results exactly as described in Theorems 2 and 3.

An alternative to the cutoff is to treat the photon as being classical, with a classical reservoir, and to study the equations of semiclassical laser theory. Then the equations of motion for the atoms remain formally unchanged, while e.g.

$$\dot{\alpha}_{(N)}(t) = -(\kappa+i\nu)\,\alpha_{(N)}(t) - i\lambda\,\omega_A^S \otimes \omega_A^R\,(\sigma^-_{(N)}(t)) + \Phi_{(N)}(t)\ . \qquad (87)$$

In reference [3] we proved both theorems without cutoffs for special sequences $\omega^S_{(N)}$ with normal fluctuations, namely coherent states of the type (30). In this case the interchange of the limit $\zeta \to \infty$ and $N \to \infty$ can be justified. We believe that Theorems 2 and 3 hold for a large class of states $\omega^S_{(N)}$ provided some uniformity properties are imposed as in (24). Theorem 1 shows that this hope is justified for the laser without reservoirs. The technical problem in generalizing Theorem 1 is to show that the covariance of the fluctuation forces $X^i_{(N)}(t)$ vanishes for $N \to \infty$.

8. CONCLUSION

From time reversible quantum dynamics we have constructed a machine which is irreversible and classical, yet displays cooperative behavior and does not necessarily tend to a state of maximum chaos. We could just as well have derived equations of motion for negative time and would have found that all the damping constants change signs. There is thus a time reversal symmetry around $t = 0$, but a break of time translation invariance. Several factors cause our system to be dissipative and self-oscillatory instead of being conservative:

(a) Coarse graining in the sense that we concentrate on very few observables, these being averages over many microscopic degrees of freedom.

(b) The limit $N \to \infty$ in a dynamical system with a mean field type of interaction.

(c) A special choice of time zero states in which the reservoirs and the system under observation are decoupled and the reservoir is in equilibrium.

The equations we have derived and their physical interpretation are not original. There is an extensive literature on the subject, with the first contribution going back to Einstein [9]. Several modern encyclopedic references are [2] and [10]. What we have demonstrated is that the irreversible and classical equations of this complex dynamical system can be derived from Hamiltonian dynamics with complete rigor and without recourse to ad hoc statistical assumptions about the nature of the influence of the reservoir on the laser proper.

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Part VI

Quantum Spin Systems

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A Proof of Part of Haldane's Conjecture on Spin Chains

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Abstract. It has been argued that the spectra of infinite length, translation and $U(1)$ invariant, anisotropic, antiferromagnetic spin s chains differ according to whether s is integral or $\frac{1}{2}$ integral: There is a range of parameters for which there is a unique ground state with a gap above it in the integral case, but no such range exists for the $\frac{1}{2}$ integral case. We prove the above statement for $\frac{1}{2}$ integral spin. We also prove that for *all* s, *finite length* chains have a unique ground state for a wide range of parameters. The argument was extended to $SU(n)$ chains, and we prove analogous results in that case as well.

1. Introduction

The spin-$\frac{1}{2}$ antiferromagnetic chain, with Hamiltonian

$$H = \sum_{i=1}^{L} [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z] \tag{1}$$

($\mathbf{S}_i^2 = \frac{3}{4}$, $\mathbf{S}_{L+1} \equiv \mathbf{S}_1$, L even) has been studied extensively. When $\Delta = 1$ it has been proven rigorously to have a unique ground state [1, 2] with a gap of $O(L^{-1})$ [2]. At $\Delta = 0$ it is equivalent to a system of massless free fermions [2]. The picture of the thermodynamic limit that emerges from the Bethe-ansatz solution and other less rigorous methods, is as follows: For $-1 < \Delta \leqslant 1$ there is a unique ground state and no gap. (For $\Delta \leqslant -1$ the system is ferromagnetic.) At $\Delta = 1$ there is Kosterlitz–Thouless transition to a doubly degenerate Néel ordered ground state with a nonzero gap. The addition of a staggered interaction

$$H \to H + \alpha \sum_{i=1}^{L} (-1)^i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{2}$$

produces a gap for $-1 < \Delta \leqslant 1$, but leaves the ground state unique.

The same behavior is expected for higher, half-integral s (i.e., $s = \frac{1}{2}, \frac{3}{2}, \ldots$) and more general interactions [nonquadratic or nonnearest neighbor]. General, isotropic, translation-invariant, antiferromagnetic Hamiltonians are expected to have a unique, gapless ground state. This phase persists for planar anisotropy ($\Delta < 1$), but a transition to a

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doubly degenerate ground state with a gap occurs for Ising anisotropy ($\Delta > 1$). Staggered interactions produce a gap, but leave the ground state unique.

Haldane has argued [3] that a quite different behavior occurs for integral s. For the Hamiltonian (1) there is a unique ground state and no gap for $-1 < \Delta \leqslant \Delta_0$ for some $\Delta_0 < 1$. At Δ_0 a Kosterlitz–Thouless transition to a phase with a unique ground state and a gap occurs. This phase persists up to some $\Delta_c > 1$ where there is an Ising transition to a double degenerate ground state, the gap vanishing only at Δ_c. Again, this behavior is expected to be generic. General Hamiltonians which are not too anisotropic are expected to have a unique ground state with a gap. Haldane's argument was based on the $s \to \infty$ limit in which a $(1+1)$-dimensional quantum field theory, the $O(3)$ nonlinear σ-model, is obtained [3, 4]. The field theory Lagrangian contains a topological angle, θ, which takes the value $\theta = 2\pi s(1+\alpha)$, for the Hamiltonian (2). When $\theta = 0$ (or a multiple of 2π) the Euclidean field theory is related to a two-dimensional classical ferromagnet at temperature $T \sim 1/s$. This theory is expected to have a gap. On the other hand, at $\theta = \pi$ the gap apparently vanishes. This picture is supported by numerical simulations [5].

In this Letter we make some of these claims rigorous. For a wide class of Hamiltonians we prove that the ground state is unique for all s for *finite* L. We are able to prove that the gap is $O(L^{-1})$ for *any* translation and $U(1)$ invariant Hamiltonian (no staggered interaction) provided that s is $\frac{1}{2}$-integral. We prove, in this case, that in the thermodynamic limit, $L \to \infty$, either there are degenerate ground states or vanishing gap. We are not able to distinguish between these two possibilities (as a function of anisotropy) except for $\Delta = 0$ and $s = \frac{1}{2}$, where there is no degeneracy. (See the remark at the end of Section 4.) Also, we are unable to prove anything about the thermodynamic limit for s integral, or with staggered interactions present. Note, however, that if our proof had worked in those cases, we would have disproved the conjecture.

Our proof relies heavily on the following fact about half-integral spin representations of $SU(2)$: If π_s is a representation with spin s, then there is an element, g, of $SU(2)$ (namely $g = -I$) such that

$$\pi_s(g) = -I, \quad (s = n + \tfrac{1}{2}). \tag{3}$$

When s is integral, (3) is false, for then $\| \pi_s(g) + I \| = 2$ for all $g \in SU(2)$. This fact is also noteworthy from the point of view that $\inf_g \| \pi_s(g) + I \|$ does not have a classical limit as $s \to \infty$.

The Haldane conjecture has been extended [4] to chains with generators of representations of $SU(n)$ on the sites, and $SU(n)$ invariant Hamiltonians. In particular, for the representation of $SU(2n)$ whose Young tableau has n rows of length m, it was argued that there is always a unique ground state, but a gap only for m even. For technical reasons, we are able to prove a unique ground state only for the case $m = 1$. However, we prove that the gap is $O(L^{-1})$ for *every* representation of $SU(n)$ (for all n) whose Young tableau has a number of boxes not divisible by n. As we shall show, the crucial property of these representations (π) is that there is a $g \in SU(n)$ such that

$$\pi(g) = zI \tag{4}$$

with $z \neq 1$. We shall show that (4) fails (with $z \neq 1$) in the contrary cases. We prove that, in the thermodynamic limit, there are either degenerate ground states or no gap for reps of $SU(2n)$ with an odd number of boxes.

We present our finite L results in Section 2 (for $SU(2)$) and Section 3 (for $SU(n)$). Our results on the thermodynamic limit ($L \to \infty$) are presented in Section 4.

2. $SU(2)$ Spin Chains

2.1. UNIQUENESS OF THE GROUND STATE

Let us begin with H in Equation (1), but with general spin s, $(\mathbf{S}_i)^2 = s(s+1)$. Let $\mathcal{S} \equiv \Sigma_i \mathbf{S}_i$. The proof [1] of a unique ground state when $\Delta = 1$ is as follows:

(i) In a particular basis, H has nonpositive off-diagonal matrix elements. This basis is the standard one in which S_i^z is specified for all i, but with the phase factor $\exp[i\pi \mathcal{S}^z_{\text{odd}}]$, where $\mathcal{S}^z_{\text{odd}} \equiv \Sigma_{i\ \text{odd}}\, S_i^z$, (and similarly for $\mathcal{S}^z_{\text{even}}$). The off-diagonal matrix elements of H come solely from the terms $S_i^+ S_{i+1}^- + h.c.$ which always change S^z_{odd} by ± 1. In this basis H is block-diagonal and the blocks are parameterized uniquely by the eigenvalues M of $\mathcal{S}^z$ (which are $M = -Ls, -Ls+1, \ldots, Ls$). In other words, any two basis vectors with a given M can be connected by sufficiently many applications of H, but two basis vectors with different M can never be connected.

(ii) By the Perron–Frobenius theorem, H has a unique ground state, $|\psi_M\rangle$, in each block and $|\psi_M\rangle$ has strictly positive entries. Note that this conclusion is independent of the nature of the diagonal elements of H. Let $E(M)$ denote the corresponding eigenvalue.

(iii) To find the absolute ground state, it is necessary to decide which $E(M)$ is the lowest. Here we use the $SU(2)$ invariance of H when $\Delta = 1$. Since $[\mathcal{S}^2, H] = 0$, each $|\psi_M\rangle$ must be an eigenfunction of $\mathcal{S}^2$. Every eigenvector with a given value of $\mathcal{S}^2$ always has, by rotation, a representative in the $M = 0$ subspace. We claim that $\mathcal{S}^2 |\psi_0\rangle = 0$, which will imply that the ground state is unique. To see this, let $|\tilde{\psi}_0\rangle$ be the unique ground state of $\tilde{H} = \mathcal{S}_{\text{odd}} \cdot \mathcal{S}_{\text{even}}$, which has $\mathcal{S}^2 |\psi_0\rangle = 0$. By the foregoing argument, $\tilde{\psi}_0$ is also positive, so $\langle \psi_0 | \tilde{\psi}_0 \rangle > 0$ and, hence, ψ_0 must have $\mathcal{S}^2 |\psi_0\rangle = 0$. Then $E(0) < E(M)$ for all $M \neq 0$. □

We present now a generalization of the foregoing theorem to a much wider class of Hamiltonians. Consider first H in (1), but with arbitrary $\Delta > -1$, for which $M = \mathcal{S}^z$ is good quantum number. By the foregoing, for every Δ the ground state in each M sector is unique. Our first new result is that *for all* $\Delta > -1$ *the ground state is uniquely* $M = 0$. The *proof* relies on the

LEMMA: *For* $\Delta > -1$ *the ground state is at most double degenerate.*

The lemma, together with $E(M) = E(-M)$, implies that the ground state is either uniquely $M = 0$ or else is a pair with M_0 and $-M_0$ for some $M_0 > 0$. In the latter case, since $E(M)$ is a continuous function of Δ, there cannot be any crossing of the $E(M_0)$ curve with any other $E(M_1)$ curve, for otherwise there would be at least a three-fold degeneracy at that Δ. But at $\Delta = 1$, $E(0) < E(M_0)$, which is a contradiction.

Proof, of Lemma: When $-1 < \Delta < 1$ make the unitary transformation $W = \exp(i(\pi/2)\mathcal{S}^x)$ so that

$$W^\dagger H W = \sum_i \tfrac{1}{4}(1+\Delta)[S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+] + \\ + \tfrac{1}{4}(1-\Delta)[S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-] + S_i^z S_{i+1}^z . \tag{5}$$

In the foregoing basis, $W^\dagger H W$ has nonpositive off diagonal elements and decomposes into precisely two connected blocks (even $\mathcal{S}^z$ and odd $\mathcal{S}^z$). For $\Delta > 1$, we replace W by $\exp(i\pi^{-1/2}\mathcal{S}^y)$. The $\Delta = 1$ case was proved previously. □

Another Hamiltonian for which the proof goes through is

$$H \to H - |J_2| \, \Sigma_i \mathbf{S}_i \cdot \mathbf{S}_{i+2} . \tag{6}$$

In general *any* spin may be coupled to any other as long as the sign is positive for odd separation and negative for even. The couplings need not be uniform. For example, the staggered coupling discussed in [3]

$$H = \sum_i [1 + \alpha(-1)^i] \, \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{7}$$

is permitted for $|\alpha| \leqslant 1$.

Nonquadratic terms are also allowed, in moderation. For example, consider a quartic term

$$\delta H = J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \tag{8}$$

$J^{-1}\,\delta H$ contains (positive) terms that change $\mathcal{S}^z_{\text{odd}}$ by ± 2. Thus, J *must* be negative. δH also has terms that change $\mathcal{S}^z_{\text{odd}}$ by ± 1 with matrix elements which, while they have nonuniform sign, are nonzero only when the corresponding elements in H are nonzero. Thus this term is alright provided J is small enough so that the negative sign for $\delta\mathcal{S}^z_{\text{odd}} = \pm 1$ coming from the quadratic term dominates. Proceeding in this way, we may add a $(\mathbf{S}_i \cdot \mathbf{S}_{i+3})^3$ term with a positive (and still smaller) coupling. We do not delineate the space of Hamiltonians with a unique ($\mathcal{S}^z = 0$) ground state; but it is clearly very large.

We note in passing that although the ground state is clearly not unique when $\Delta \leqslant -1$, the foregoing proves that it *is* unique if H is restricted to the $S^z = 0$ sector.

2.2. INFINITESIMAL ENERGY GAP

We now turn to our second result concerning the excitation energy. Following [2] we construct a state orthogonal to the ground state and with energy $O(L^{-1})$. The state is $|\psi\rangle = U|\psi\rangle$, where $|\psi\rangle$ is the unique ground state and U is a unitary operator which rotates all spin about the z-axis by a slowly varying amount.

$$U = e^A , \quad A = \frac{2i\pi}{L} \sum_{j=1}^{L} j S_j^z .$$

We may assume the ground state is unique, since, if not, the gap is precisely zero. Note that the final, Lth, spin is unrotated so that the relative rotation between $\mathbf{S}_L$ and $\mathbf{S}_1$ is also small.

To calculate the energy, note that

$$\begin{aligned} U^\dagger \mathbf{S}_i \cdot \mathbf{S}_{i+1} U - \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ = (1/2)\sin(2\pi/L)\,(\mathbf{S}_i \times \mathbf{S}_{i+1})_z + \\ + [\cos(2\pi/L) - 1]\,(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - S_i^z S_{i+1}^z)\,. \end{aligned} \tag{9}$$

Let $C = \frac{1}{2}\sin(2\pi/L)\Sigma_i(\mathbf{S}_i \times \mathbf{S}_{i+1})_z$. Although it would appear that $\langle\psi|\, C\,|\psi\rangle$ is $O(1)$, we note that C = (const.) $[H, A]$ and, hence, $\langle\psi|\, C\,|\psi\rangle = 0$ in any eigenstate of H. Thus,

$$\begin{aligned} \delta E &= \langle\psi|\, U^+ HU - H\,|\psi\rangle \\ &= [\cos(2\pi/L) - 1] \sum_i \langle\psi|\, S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\,|\psi\rangle = O(L^{-1})\,. \end{aligned} \tag{10}$$

This proof extends trivially to the wider class of Hamiltonians considered above. Clearly a nonisotropic $S_i^z S_{i+1}^z$ coupling changes nothing. An mth neighbor coupling, $H_m \propto \Sigma_i \mathbf{S}_i \cdot \mathbf{S}_{i+m}$, or quartic couplings as in (8), have the property that if we write $U^\dagger HU - H = C + D$, as in (9) then, although $C \neq$ (const.) $[H, A]$, it is true that C = const. $[H, A] + O(L^{-1})$.

It is to be noted that our proof that $\delta E = O(L^{-1})$ does not use any invariance properties of H and is applicable to *all* $\Delta \in (-\infty, \infty)$.

The crucial point, which we now address, is that $\langle\psi|\, U\,|\psi\rangle = 0$, and thus that δE really is an upper bound to the excitation energy. The proof of this [2] requires translation and $U(1)$ invariance of H. It works for all $\Delta \in (-\infty, \infty)$. Let T be the operator of translation by one site. Then, by uniqueness of ψ, $T\,|\psi\rangle = e^{i\alpha}\,|\psi\rangle$ for some α, $\mathscr{S}^z\,|\psi\rangle = 0$, and

$$\begin{aligned} \langle\psi\,|U\,|\psi\rangle &= \langle\psi|\, TUT\,|\psi\rangle = \langle\psi|\exp\left(i\,\frac{2\pi}{L}\sum_{i=1}^{L} iS_{i+1}^z\right)|\psi\rangle \\ &= \langle\psi|\, U\exp(2i\pi S_1^z)\exp\left(-i\,\frac{2\pi}{L}\,\mathscr{S}^z\right)|\psi\rangle \\ &= \langle\psi|\, U\exp(2\pi i S_1^z)\,|\psi\rangle\,. \end{aligned} \tag{11}$$

The operator $\exp(2i\pi S_1^z)$ is $\pm I$ for s integer or half-integer, giving

$$\langle\psi|\, U\,|\psi\rangle = \pm\,\langle\psi|\, U\,|\psi\rangle \quad \begin{pmatrix} s \text{ integral} \\ s \text{ half-integral} \end{pmatrix}. \tag{12}$$

Although (12) is not very interesting in the integral case, it proves that $\langle\psi|\, U\,|\psi\rangle = 0$ for s half-integral and $\Delta > -1$. We used a fundamental property of half-integer spin states, namely (3).

This proof generalizes immediately to all Hamiltonians considered above, except the nonuniform ones. In particular, it does not work for alternating interactions. One could try repeating the proof with T the generator of translations by two sites in which case (11) becomes

$$\langle \psi | U | \psi \rangle = \langle \psi | U \exp(2i\pi(S_1^z + S_2^z)) | \psi \rangle .$$

But $\exp(2i\pi(S_1^z + S_2^z))$ is I for S integer or half-integer so the proof fails. This is also in accord with the Haldane conjecture.

3. $SU(n)$ Chains

Instead of generators, S, of the spin-s representations of $SU(2)$, we place generators of a representation of $SU(n)$ on each site. We use the same representation on each site. This insures translation invariance, which was a crucial element in the previous $SU(2)$ proof. Unlike the $SU(2)$ case, there are representations of $SU(n)$ that are not self-conjugate, which means that a nearest neighbor pair of 'spins' cannot form a singlet state. [For such nonself-conjugate representations there is another way to put $SU(n)$ on the lattice, namely alternate the representation and its conjugate. This is considered in [4]. Our proof of the infinitesimal gap fails in these cases for want of translation invariance.] Of particular physical interest are the self-conjugate representations of $SU(2n)$ whose Young tableaux have n rows, each of length m. [For $SU(2)$, spin-s corresponds to one row of length $2s$.] The Haldane conjecture was extended to this case [4]: an energy gap is predicted for m even, but not odd.

We prove uniqueness of the ground state for $SU(2n)$ with the antisymmetric n-tensor representation (i.e., $m = 1$ above). Under the *assumption* of a unique ground state (which must be an $SU(n)$ singlet) we extend our proof of infinitesimal energy gap to all representations of $SU(n)$ whose Young tableaux contain a number of boxes not divisible by n. [Of course, if the ground state is not unique the gap is exactly zero.]

3.1. UNIQUENESS OF THE GROUND STATE: $SU(2n)$, $m = 1$

The state at each site is labelled by n different integers $1 \leqslant i_1, i_2, \ldots, i_n \leqslant 2n$. We may think of these as labelling the 'flavors' of n fermions inhabiting that site. Anti-symmetry is enforced by fermi statistics. There are $2n$ flavors in total. Taking a (non-Hermitean) basis of operators S_j^i, $i, j = 1, \ldots, 2n$ such that

$$[S_j^i, S_l^k] = \delta_l^i S_j^k - \delta_j^k S_l^i ,$$

$$S_j^{i\dagger} = S_i^j, \; S_i^i = 0 \quad \text{(repeated indices summed)} \tag{13}$$

we may write

$$S_j^i = \psi^{\dagger i}\psi_j - \tfrac{1}{2}\delta_j^i , \tag{14}$$

where $\psi_i(\psi^{\dagger i})$ annihilates (creates) a fermion of flavor i. The total number of fermions

(on all sites) of each flavor

$$\sum_{k=1}^{L} \psi_k^{\dagger i} \psi_{i,k} = N_i \tag{15}$$

is conserved. The simple, quadratic Hamiltonian is

$$H = \sum_{k=1}^{L} S_{j,k}^{i} S_{i,k+1}^{j} = \sum_{k=1}^{L} \psi_k^{\dagger i} \psi_{j,k} \psi_{k+1}^{\dagger j} \psi_{i,k+1} + \text{constant} \tag{16}$$

with L even. H simply exchanges flavors of two fermions on adjacent sites. We again wish to argue that, in some basis, H has nonpositive off-diagonal matrix elements. We define this basis by assigning phases, ± 1, to the states described above. This phase is given by the sign of a certain permutation of the numbers $1, 2, 3, \ldots, nL$. Consider the nL fermions to lie along a straight line, all at different points, by arbitrarily ordering the fermions on a given site. The permutation is determined by indexing the N_1 flavor 1 fermions from left to right on the lattice $(1, 2, \ldots, N_1)$ then indexing flavor 2 fermions $(N_1 + 1, \ldots, N_1 + N_2)$, etc. Note that this phase correctly accounts for the antisymmetry under permutation of the fermions on a given site. We now must show that the nondiagonal terms in H change the sign of this permutation. Suppose that H switches a flavor i fermion on site k with a flavor j fermion on site $k + 1$. The initial and final states are only possible if there are no other i's or j's on either site. Thus the only effect is to transpose the indices of these two fermions and this changes the sign of the permutation.

Next we must prove the connectedness property. This follows because we may permute fermions down the lattice until we achieve any desired configuration on the first site, then the second site, etc., subject only to the constraint on the total number of fermion of each flavor. Next, we argue that the ground state in the *symmetric sector* of the Hilbert space (the analogue of the $\mathcal{S}^2 = 0$ sector in the $SU(2)$ case) in which all N_i are equal is the overall ground state. This will follow if we can prove that the ground state in any other sector has a degenerate partner in the symmetric sector. Such a partner can always be constructed by applying the 'raising operator' $\mathcal{S}_j^i = \Sigma_k S_{j,k}^i$, which commutes with H, raises N_i by one and lowers N_j by one. Finally to prove that the unique ground state in the symmetric sector is an $SU(2n)$ singlet we observe that it has nonzero overlap with the singlet ground state of the trivial Hamiltonian with decoupled neighboring pairs.

This proof extends straightforwardly to other antisymmetric tensor representations but not to Young tableaux with more columns. Nonetheless, it seems reasonable that the ground state should be a singlet for some wide class of such Hamiltonians.

3.2. INFINITESIMAL ENERGY GAP

We now prove that the energy gap is $O(L^{-1})$ for all representations of $SU(n)$ [with the same representation on each site] except those whose Young tableaux have integer multiples of n boxes. Generalizing the $SU(2)$ case, we consider a slowly varying

'rotation' of the generators:

$$U = e^{A}, \quad A = 2\pi i \sum_{k=1}^{L} kQ_k/L . \tag{17}$$

Here Q in some element of the Lie algebra of the representation (the same for each site). In order that the 'rotated' state $U|\psi\rangle$ have an infinitesimal energy gap we require that

$$\exp(-2\pi i Q_L) S^i_{j,L} \exp(2\pi i Q_L) = S^i_{j,L}, \ \forall ij . \tag{18}$$

By Schur's Lemma, (18) implies

$$\exp(2\pi i Q) = zI . \tag{19}$$

To calculate the excitation energy, write $H = \Sigma_{k=1}^{L} H_k$, with $H_k = S^i_{j,k} S^j_{i,k+1}$, and note that

$$U^{\dagger} H_k U = \exp\left[-\frac{i\pi}{L}(Q_{k+1} - Q_k)\right] H_k \exp\left[\frac{i\pi}{L}(Q_{k+1} - Q_k)\right]$$

since

$$[H_k, (Q_{k+1} + Q_k)] = 0 .$$

But then

$$U^{\dagger} H U - H = \frac{i\pi}{L} \sum_{k=1}^{L} [H_k, (Q_{k+1} - Q_k)] + O(L^{-1}) . \tag{20}$$

The commutator in (20) is $[H, A]$ and so has vanishing expectation in any eigenstate of H.

To prove orthogonality with the ground state we again use the assumed uniqueness and observe, as in (11), that

$$\langle\psi| U |\psi\rangle = \langle\psi| TUT |\psi\rangle$$

$$= \langle\psi| U \exp\left[-(2\pi i/L) \sum_{k=1}^{L} Q_k + 2\pi i Q_1\right] |\psi\rangle = z \langle\psi| U |\psi\rangle . \tag{21}$$

Thus $\langle\psi| U |\psi\rangle = 0$ if we can find a $g \in SU(n)$ obeying

$$\pi(g) = \exp(2\pi i Q) = zI, \quad \text{with } z \neq 1 .$$

In (21) we used the fact that $\Sigma\, Q_k |\psi\rangle = 0$ since $|\psi\rangle$ is $SU(n)$ invariant. If we choose $g = e^{2\pi i/n} I$, then $\pi(g) = e^{2\pi i B/n} I$, where B is the number of boxes in the tableau. Thus $z \neq 1$, provided $B/n \notin \mathbf{Z}$. On the other hand, if $B/n \in \mathbf{Z}$ no choice of g gives $z \neq 1$ since $\pi(g) = I$ for all elements of the center, $Z(n)$, of $SU(n)$, but $SU(n)/Z(n)$ is a simple Lie group and thus contains no element, G, obeying $\pi(G) = zI$ with $z \neq 1$. [If such elements existed they would generate a normal subgroup.] Specializing to reps of $SU(2n)$ whose

tableaux have n rows of length m, our proof works only when m is odd. This supports the conjecture of [4]. The proof does *not* work for Hamiltonians with a representation and its (inequivalent) conjugate on alternating sites since we then have symmetry only under translation by two sites and Equation (21) is replaced by

$$\langle \psi | U | \psi \rangle = \langle \psi | U \exp 2\pi i(Q_1 - Q_2') | \psi \rangle = \langle \psi | U | \psi \rangle . \tag{22}$$

If we consider equivalent reps on each site, but alternating interaction strength, we obtain

$$\langle \psi | U | \psi \rangle = \langle \psi | U \exp 2\pi i(Q_1 + Q_2) | \psi \rangle . \tag{23}$$

In this case the proof works when *twice* the number of boxes is not divisible by n. So the proof fails with alternating interaction strength for the reps of $SU(2n)$ with n rows of length m, for m even *or* odd, again supporting the conjecture of [4].

4. Thermodynamic Limit

So far we have proved the following for finite L in a variety of cases: (i) The ground state is unique; (ii) The gap is $O(L^{-1})$. Unfortunately, uniqueness of the ground state for finite L does not imply uniqueness when $L = \infty$. As an example of what can go wrong consider $s = \frac{1}{2}$ and $\Delta \gg 1$. Roughly, $|\psi\rangle \simeq 2^{-1/2}(|\psi_+\rangle + |\psi_-\rangle)$, with $|\psi_-\rangle = + - + - \cdots$ and $|\psi_+\rangle = - + - + \cdots$ being Néel states. Then $U|\psi\rangle \simeq i2^{-1/2}(|\psi_+\rangle - |\psi_-\rangle)$ which, for finite L, has slightly higher energy. But as $L \to \infty$, $|\phi_\pm\rangle = 2^{-1/2}(|\psi\rangle \pm iU|\psi\rangle)$ can become two decoupled ground states (i.e., $\langle \phi_- | a | \phi_+ \rangle = 0$ for all local operators, a). According to the discussion in Section 1, this phenomenon does occur if and only if $\Delta > 1$ for $\frac{1}{2}$ integral spin.

Let us be precise about the definitions of ground state and gap when $L = \infty$. Let $\mathscr{A}$ denote the local algebra of observables and $\mathscr{A}^q$ the quasi-local algebra (norm closure of $\mathscr{A}$). ρ denotes a state on $\mathscr{A}^q$ (with $\rho(a^\dagger a) \geqslant 0$ and $\rho(I) = 1$). H^L and E^L denote the Hamiltonian and ground state energy for a (periodic) system of finite length L. For $\alpha \in \mathscr{A}$,

$$a^L(t) \equiv \exp(iH^L t) a \exp(-iH^L t)$$

and

$$a(t) = \underset{L \to \infty}{\text{norm-lim}}\, a^L(t) \tag{24}$$

exists [6] uniformly on intervals $t \in [-T, T]$. (We would get the same $a(t)$ in (24) if we used H^L with free, instead of periodic boundary conditions.) Hence, $a(t)$ is defined for $a \in \mathscr{A}^q$.

DEFINITION. ρ is a *ground state for the infinite system* if, for all $a, b \in \mathscr{A}^q$, $f_{ab}(t) \equiv \rho(ab(t))$ satisfies $\operatorname{supp} \hat{f}_{ab} \subset [0, \infty)$, where $\hat{f}$ is the (distributional) Fourier transform of f.

For another definition of ground state, see [7].

DEFINITION. ρ has a *gap* w_0 if, for all $a, b \in \mathscr{A}^q$, supp $\hat{f}_{ab} \cap (0, w_0)$ is empty.

Let $|\psi^L\rangle$ denote a ground state for H^L. In many cases we proved it is unique, but that fact will not be used here. A ground state ρ can be constructed as

$$\rho(a) = \lim_{L\to\infty} \langle \psi^L | a | \psi^L \rangle$$

for $a \in \mathscr{A}$ (and by passing to a subsequence if necessary).

THEOREM. *Let* $U \in \mathscr{A}$ *and* $\varepsilon > 0$ *be fixed and satisfy (for all sufficiently large* $L > |\text{supp } U|$)

(a) $\langle \psi^L | U^\dagger U | \psi^L \rangle \geqslant 1$,

(b) $\langle \psi^L | U^\dagger (H^L - E^L) U | \psi^L \rangle \leqslant \varepsilon$,

(c) $\langle \psi^L | U | \psi^L \rangle = 0$.

Then, either (a) *there is more than one ground state or* (b) *there is only one ground state* ρ *with gap* $w_0 \leqslant \varepsilon$.

We shall apply the theorem to $SU(2)$ (s half-integral) and $SU(2n)$ (for reps with an odd number of boxes). The U given in Sections 2 and 3 is not applicable here (since it depends on L) and we shall construct a suitable L independent U later.

Sketch of Proof. Suppose ρ is unique with gap $w_0 > \varepsilon$. We want to find a contradiction. Let $\varepsilon < \tilde{w}_0 < w_0$. Let $\hat{g}(w) \in C_0^\infty$ with

$$0 \leqslant \hat{g}(w) \leqslant 1\,, \quad \hat{g}(w) = \hat{g}(-w)\,, \quad \hat{g}(w) = 1$$

for

$$|w| < \tfrac{2}{3}\varepsilon + \tfrac{1}{3}\tilde{w}_0\,, \quad \hat{g}(w) = 0$$

for $|w| \geqslant \tilde{w}_0$. Then $g(t) = g(-t) =$ real and $g(t)$ is in Schwartz space, so with

$$K^L = \int g(t) U^L(t)\,, \quad K \equiv \operatorname*{norm\text{-}lim}_{L\to\infty} K^L \in \mathscr{A}^q\,.$$

The uniform convergence of $b^L(t) \to b(t)$ implies

$$\lim_{L\to\infty} \langle \psi^L | ab^L(t) | \psi^L \rangle = \rho(ab(t)) \quad \text{for all } a, b \in \mathscr{A}\,.$$

Pick $0 < \delta < \varepsilon$ and let Δ^L (resp. π^L) $\equiv$ spectral projection of $H^L - E^L$ on $[0, \delta)$ (resp. $[\delta, \tilde{w}_0]$). $\Gamma^L \equiv \pi^L + \Delta^L$. The gap condition implies for all $a, b \in \mathscr{A}$

$$\langle \psi^L | a\pi^L b^L(t) | \psi^L \rangle \to 0\,. \tag{25}$$

By (b),

$$\varepsilon \geqslant \langle \psi^L | U^\dagger (H^L - E^L) U | \psi^L \rangle \geqslant \tilde{w}_0 \langle \psi^L | U^\dagger (1 - \Gamma^L) U | \psi^L \rangle\,,$$

so

$$\langle \psi^L | U^\dagger \Gamma^L U | \psi^L \rangle \geqslant (\tilde{w}_0 - \varepsilon)/\tilde{w}_0\,.$$

By (25)

$$\liminf_{L\to\infty} \langle \psi^L | U^\dagger \Delta^L U | \psi^L \rangle \geqslant (\tilde{w}_0 - \varepsilon)/\tilde{w}_0 .$$

Let

$$Z \equiv \rho(K^\dagger K) = \lim_{L\to\infty} \langle \psi^L | U^\dagger [\hat{g}(H^L - E^L)]^2 U | \psi^L \rangle$$

$$\geqslant \lim_{L\to\infty} \langle \psi^L | U^\dagger \Delta^L U | \psi^L \rangle \geqslant (\tilde{w}_0 - \varepsilon)/\tilde{w}_0 .$$

Further, since supp $\hat{g} \in [-\tilde{w}_0, \tilde{w}_0]$,

$$K^L | \psi^L \rangle = \Gamma^L K^L | \psi^L \rangle . \tag{26}$$

Let $v(a) = Z^{-1}\rho(K^\dagger a K)$. We claim that v is a ground state. From (26)

$$f_{ab}(t) \equiv v(ab(t)) = Z^{-1} \lim_{L\to\infty} \langle \psi^L | K^{L\dagger} ab(t) (\pi^L + \Delta^L) K^L | \psi^L \rangle .$$

By the Schwarz inequality, the π^L term can be bounded by

$$\langle \psi^L | K^{L\dagger} ab(t) b^\dagger(t) a^\dagger K^L | \psi^L \rangle^{1/2} \langle \psi^L | K^{L\dagger} \pi^L K^L | \psi^L \rangle^{1/2} .$$

The first factor is bounded and the second goes to zero by (25). Then,

$$f_{ab}(t) = Z^{-1} \lim_{L\to\infty} \langle \psi^L | ab(t) \Delta^L K^L | \psi^L \rangle ,$$

and therefore supp $\hat{f}_{ab} \subset [-\delta, \infty)$. But δ was arbitrary, so supp $f_{ab} \subset [0, \infty)$.

For $\lambda \in \mathbf{C}$ consider the state $\mu_\lambda(a) = (1 + |\lambda|^2 Z)^{-1} \rho((1 + \lambda^* K^\dagger) a (1 + \lambda K))$. (This is correctly normalized since $\rho(K) = \lim_{L\to\infty} \int \langle \psi^L | U | \psi^L \rangle g = 0$ by (c).) By the above proof $\rho(K^\dagger ab(t) K)$ satisfies the spectral condition and so does $\rho(ab(t)K)$. Also, $\rho((K^\dagger a) b(t))$ does too (since ρ is a ground state). Thus μ_λ is a ground state. By the assumed uniqueness, $\mu_i = \mu_{-i} = \mu_1 = \mu_{-1} \Rightarrow \rho(aK) = 0$ for all a. But $\rho(K^\dagger K) \neq 0$, which is a contradiction. □

Our next goal is to construct U satisfying the hypotheses of the theorem. If we can make ε arbitrarily small the Haldane conjecture will have been proved for s half-integral ($SU(2)$) or for an odd number of boxes ($SU(2n)$). The U in Sections 2 and 3 covered more cases (and that is why it was presented) but for this theorem we need an L independent U. For $SU(2)$, let

$$U_l = \exp\left\{ \frac{i\pi}{l} \sum_{j=-l}^{l} S_j^z (j + l) \right\}, \tag{27}$$

which is unitary. It is easy to check, as before, that (b) is satisfied with $\varepsilon = O(l^{-1})$. Here H^L is any translation invariant Hamiltonian considered in Section 2. Introduce the unitary R by

$$R(S_j^x, S_j^y, S_j^z) R^{-1} = (-S_{-j}^x, S_{-j}^y, -S_{-j}^z) . \tag{28}$$

Then, for all Δ, $RH_L R^{-1} = H_L$, $R^2 = I$ and thus $R\,|\psi^L\rangle = \pm\,|\psi^L\rangle$. [Note that, even if the ground state for finite L is not unique, a ground state can be chosen obeying this equation.] Moreover,

$$RU_l R^{-1} = \pm U_l \begin{pmatrix} s \text{ integral} \\ s \text{ half-integral} \end{pmatrix}. \tag{29}$$

Consequently, $\langle \psi^L |\, U_l \,| \psi^L \rangle = 0$ for s half-integral. Since l is arbitrary, there is no gap.

This construction of U_l extends to those representations of $SU(2n)$ with an odd number, B, of boxes in their Young tableaux. (Recall that we proved an infinitesimal energy gap for a bigger class, namely reps of $SU(n)$ with B not divisible by n.) We take

$$U_l = \exp\left[\frac{i\pi}{l} \sum_{j=-l}^{l} Q_j (j+l)\right] \tag{30}$$

where $Q = \pi(q)$ and q is in the Lie algebra of $SU(2n)$. To imitate the $SU(2)$ construction, we require $\exp(2i\pi Q) = zI$, $z \neq 1$, and $V \in SU(2n)$ such that $VqV^{-1} = -q$. One choice is

$$q = \frac{1}{2}\begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix}, \qquad V = \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix} \Rightarrow \exp(2i\pi q) = -I$$

and

$$\exp(2i\pi Q) = (-1)^B I = -I.$$

Let T be the reflection unitary: $TQ_j T^{-1} = Q_{-j}$. Then $R \equiv T \prod_{k=1}^{L} \pi(V_i)$ satisfies (29) and $|\psi^L\rangle$ can be chosen so that $R\,|\psi^L\rangle = \pm\,|\psi^L\rangle$.

Remark. The theorem, together with our construction of U_l, proves the Haldane conjecture for H in (1) for $\Delta > -1$ and s half-integral, in the sense that a unique ground state and a gap cannot coexist when $L = \infty$. The reader may well ask whether it is known rigorously for *any* Δ that the ground state is unique. Araki and Matsui [8] have proved the uniqueness for the special case $\Delta = 0$ and $s = \frac{1}{2}$. In fact they have shown more. They consider

$$H = \sum_{i=1}^{L} (1+\gamma) S_i^x S_{i+1}^x + (1-\gamma) S_i^y S_{i+1}^y + h S_i^z \tag{31}$$

and prove the following for $|h| < 2$: (i) if $\gamma = 0$, the ground state is unique and there is no gap. (ii) If $1 > |\gamma| > 0$ there are exactly two pure ground states, and the results in the paper can be used to show that both states have a gap [9].

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Note added in proof. Results similar to some of those presented here were obtained by M. Kolb, *Phys. Rev.* **D31**, 7494 (1985).

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Rigorous Results on Valence-Bond Ground States in Antiferromagnets

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We present rigorous results on a phase in antiferromagnets in one dimension and *more*, which we call a valence-bond solid. The ground state is simply constructed out of valence bonds, is nondegenerate, and breaks no symmetries. There is an energy gap and an exponentially decaying correlation function. Physical applications are mentioned.

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There is currently considerable interest in the ground-state properties of quantum antiferromagnets. In the one-dimensional case, it has been argued by Haldane[1] that Heisenberg antiferromagnets have an energy gap for integer, but not half-odd-integer, spin. Neutron-scattering data on $CsNiCl_3$, a highly one-dimensional spin-1 antiferromagnet, support this claim.[2] It has also been argued by Anderson[3] that two-dimensional antiferromagnets can have disordered ground states. The nature of these ground states may be important in the theory of high-T_c superconductors.[4]

A convenient basis for spin-singlet states of a spin $s=\frac{1}{2}$ antiferromagnet consists of all possible products of pairwise contractions of spins to form singlets (known as valence bonds): $(\uparrow\downarrow-\downarrow\uparrow)$. For an $s=\frac{1}{2}$ chain with a special ratio of first and second nearest-neighbor interactions it was shown by Majumdar and Ghosh[5] that the two exact ground states are given by the states with purely nearest-neighbor valence bonds. We represent these dimerized states in Fig. 1 by drawing lines between the pairs of spins which are contracted. These ground states have a translational symmetry broken from period 1 to period 2, ultrashort-range correlations, and, as we will prove in a companion paper,[6] an energy gap. The pure nearest-neighbor model, which was solved by the Bethe *Ansatz*, is believed to have a unique ground state with power-law correlations and no gap. This ground state can be thought of as a resonating-valence-bond state[3] in which quantum fluctuations restore the translational symmetry and mix in bonds of greater length. The absence of Néel order is believed to be a general feature of one-dimensional antiferromagnets. On the other hand, Néel order is generally expected to occur in two (or more) dimensions at zero temperature. However, it was suggested[3] that a disordered resonating-valence-bond ground state might occur in some two-dimensional $s=\frac{1}{2}$ cases: triangular lattice or square lattice with next-neighbor couplings. The latter is relevant to the copper-oxide planes in high-T_c superconductors.[4]

FIG. 1. The spin-$\frac{1}{2}$ dimerized valence-bond states.

In this Letter and the companion paper,[6] we will study exactly solvable Hamiltonians, in dimension one *and more*, with ground states constructed simply out of valence bonds, which have quite a different character than the Majumdar-Ghosh model. Unlike the dimerized ground states of Ref. 5, our models have unique ground states with no broken symmetries. As in the model of Ref. 5 there is a gap and short-range correlations. *This ground state, which we call a valence-bond solid (VBS)*, appears to be a good approximation to the ground state of the realistic spin-1 chain. We suspect that it may be a good approximation in other physically relevant cases as well. The existence of a short-range, nondegenerate phase in antiferromagnets was first suggested, for the one-dimensional case, by Haldane.[1] We present the first exact solution exemplifying this phase in one dimension, and extend the results to higher dimension.

We extend the notion of valence bonds in a natural way to higher spin. Spin s is obtained by symmetrization of $2s$ spin-$\frac{1}{2}$ variables. Thus, any spin-singlet state can be written with $2s$ valence bonds emanating from each site and terminating on different sites. (The symmetrization implies that we do not distinguish the $2s$ different bonds ending at a given site.)

Our simplest model, and the one with which we will be the most concerned, is an $s=1$ chain. We first present the ground state and then give the Hamiltonian. The VBS ground state is the (unique) state with a single valence bond connecting each nearest-neighbor pair of spins (see Fig. 2). This state was first introduced (as far as we know) in the discussion of the large-n limit of $SU(n)$ chains.[7] Note that, unlike in the dimerized $s=\frac{1}{2}$ ground state,[5] the translational symmetry is unbroken. To find a Hamiltonian for which this is the ground state, note that the presence of a valence bond between each

FIG. 2. The spin-1 valence-bond-solid state.

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neighboring pair implies that the total spin of each such pair cannot be 2. (After contracting two of the $s=\frac{1}{2}$ variables to form a singlet, the remaining $s=\frac{1}{2}$'s could form either a triplet or a singlet.) Thus, we choose our Hamiltonian to be a sum of projection operators onto spin 2 for each neighboring pair:

$$H=\sum_i P_2(\mathbf{S}_i+\mathbf{S}_{i+1})$$
$$=\sum_i[\tfrac{1}{2}\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{1}{6}(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2+\tfrac{1}{3}]. \quad (1)$$

Clearly, the ground-state energy is zero. We will calculate the exact ground-state correlation function below and prove the existence of a gap in Ref. 6. For a finite chain with open boundary conditions, there are several ground states, but we will prove in Ref. 6 that there is a unique ground state in the infinite-volume limit.

Various generalizations of this model immediately suggest themselves. The most interesting one is perhaps an $s=\frac{3}{2}$ anitferromagnet on a hexagonal (honeycomb) lattice. The VBS ground state has a single valence bond connecting each neighboring pair. The Hamiltonian is a projection operator onto spin 3 for each neighboring pair. The VBS state has no projection onto spin 3 for any pair because two of the six effective spin $\frac{1}{2}$'s on each pair of sites are contracted to form a singlet, allowing a maximum possible spin of 2. We will prove in Ref. 6 that the correlation function decays exponentially for this model. This implies that the ground state is not Néel ordered. We believe that there is a unique ground state in this model in the infinite-volume limit and that there is a gap, but we are unable to prove either of these conjectures. In general, there is a solvable model with a VBS ground state whenever $2s$ equals the coordination number of the lattice. The ground state has one valence bond on each lattice link and the Hamiltonian projects out spin $2s$ for each neighboring pair. More generally, there are solvable models with $2s$ equal to an integer multiple, n, of the coordination number, the ground state now containing n valence bonds on each lattice link. The Hamiltonian is a sum of projection operators for pairs of neighboring spins, onto spin $s'>2s-n$, with positive coefficients:

$$H=\sum_{\langle ij\rangle}\sum_{s'=2s-n+1}^{2s} a_{S'}P_{S'}(\mathbf{S}_i+\mathbf{S}_j), \quad (2)$$

with all $a_{S'}>0$. We refer to such a ground state as a valence-bond solid because the valence-bond structure mimics the lattice. This state can only exist if the lattice type and spin magnitude are commensurate in the way described above.

On the basis of the rigorous results mentioned above for $s=1$ in one dimension and $s=\frac{3}{2}$ on a hexagonal lattice, it is tempting to conclude that VBS states might generally have exponential decay, a gap, and no Néel order. However, this may not be the case in general. We will show[6] that the VBS state on a Cayley tree actually *has* Néel order for sufficiently large coordination number. Thus, we might expect Néel order for regular lattices of sufficiently high coordination number and dimension. We will relate this issue to the properties of certain random walks on the same lattice.[6] We generally refer to the VBS *phase* as the phase with a unique ground state, exponential decay, a gap, and no Néel order. We expect that it occurs for a range of Hamiltonians including the solvable ones and, in one dimension, the realistic ones. By the VBS *state*, we mean the state constructed simply out of valence bonds, as described above. With this terminology some Hamiltonians with a VBS *ground state* may not be in the VBS *phase*.

Other simple valence-bond ground states also exist which, unlike the VBS state, have only a period-2 translational symmetry. We will generally refer to these as dimerized ground states. The simplest example is the $s=\frac{1}{2}$ chain of Majumdar and Ghosh[5]:

$$H=\sum_i P_{3/2}(\mathbf{S}_i+\mathbf{S}_{i+1}+\mathbf{S}_{i+2})$$
$$=\tfrac{4}{3}\sum_i[\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\tfrac{1}{2}\mathbf{S}_i\cdot\mathbf{S}_{i+2}+\tfrac{3}{8}], \quad (3)$$

where $P_{3/2}$ projects onto spin $\frac{3}{2}$. The dimerized states of Fig. 1 have neighboring pairs of spins combined to form a singlet, and therefore each group of three neighboring spins is in an $s=\frac{1}{2}$ state.

This model has a direct generalization for arbitrary spin.[8] For an $s=1$ chain, a solvable Hamiltonian is a sum of projection operators onto spin 0, 2, and 3, with positive coefficients, for each group of three neighboring spins. The dimerized states with double valence bonds between pairs of neighboring spins (see Fig. 3) are ground states, since two of the spins in each group of three neighboring spins are contracted to form a singlet so that the total spin of the three spins is necessarily 1. The VBS state is *not* a ground state in this case, since in that state groups of three neighboring spins have a projection onto $s=0$. We expect that the two dimerized states are the only ground states. This construction generalizes to arbitrary spin s.[8] H is a sum of projections onto all spins but s, with positive coefficients, for each group of three neighboring spins. The ground state has $2s$ valence bonds on every second link.

There also exist Hamiltonians with partially dimerized ground states. Two such states for an $s=\frac{3}{2}$ chain are shown in Fig. 4. To construct a Hamiltonian for which these are the ground states, we begin with the sum of the projections onto $s=\frac{5}{2}$, $\frac{7}{2}$, and $\frac{9}{2}$ for each group of three neighboring spins. The states in Fig. 4 are ground states, since each group of three neighboring spins contain three

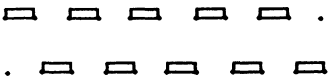

FIG. 3. The spin-1 dimerized states.

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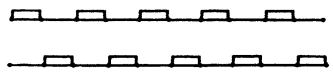

FIG. 4. The spin-$\frac{3}{2}$ partially dimerized states.

valence bonds and so have a maximum spin of $s=\frac{3}{2}$. The fully dimerized states which alternate between three and zero valence bonds between adjacent sites are also ground states. We expect that these fully dimerized ground states can be eliminated by adding to the Hamiltonian the projection onto $s=3$ for each pair of adjacent spins.

We now outline the calculation of the exact correlation function for the $s=1$ VBS model (more details will be given in Ref. 6). We label the two states of a spin-$\frac{1}{2}$ variable as ψ_α, where $\psi_1=(+)$ and $\psi_2=(-)$, and $\{(+),(-)\}$ is the standard S_z eigenstate basis. We will define a *raised* index by multiplication by ϵ: $\psi^\alpha\equiv\epsilon^{\alpha\beta}\psi_\beta$. Here $\epsilon^{\alpha\beta}$ is the antisymmetric tensor with $\epsilon^{12}=1$, and we use a summation convention for repeated indices. The Hermitian-conjugate state to ψ_α will be defined with a raised index $\psi^{\dagger\alpha}$. The normalization is given by $\psi^{\dagger\alpha}\psi_\beta=\delta^\alpha_\beta$, where δ^α_β is the Kronecker-δ tensor, the unit matrix. A valence bond between two spins corresponds to the state $\psi^\alpha\otimes\psi_\alpha$.

Our notation for higher spin is based on the representation of spin s as $2s$ symmetrized spin-$\frac{1}{2}$ variables. Thus, we write a spin-1 variable as $\psi_{\alpha\beta}=(\psi_\alpha\otimes\psi_\beta+\psi_\beta\otimes\psi_\alpha)/\sqrt{2}=\psi_{\beta\alpha}$. The VBS state for an open chain of N spins is

$$\chi^{\alpha_{N+1}}_{\alpha_1}=\psi_{\alpha_1\alpha_2}\otimes\psi^{\alpha_2\alpha_3}\otimes\psi_{\alpha_3\alpha_4}\otimes\psi^{\alpha_4\alpha_5}\otimes\cdots\otimes\psi^{\alpha_N\alpha_{N+1}},$$

where the pairs of symmetrized indices label the spin-1 variables along the chain. The basic result needed to obtain the correlation function is the ground-state normalization, $\chi^{\dagger\beta_1}_{\beta_{N+1}}\chi^{\alpha_{N+1}}_{\alpha_1}$. This is given by a product of N factors $(\delta^{\alpha_i}_{\beta_i}\delta^{\alpha_{i+1}}_{\beta_{i+1}}+\delta^{\alpha_i}_{\beta_{i+1}}\delta^{\alpha_{i+1}}_{\beta_i})$. Expanding the N factors and contracting all indices gives a geometrical sum which can be evaluated exactly, giving

$$\chi^{\dagger\beta_1}_{\beta_{N+1}}\chi^{\alpha_{N+1}}_{\alpha_1}=\frac{3^N-1}{2}\delta^{\beta_1}_{\alpha_1}\delta^{\alpha_{N+1}}_{\beta_{N+1}}+\delta^{\beta_1}_{\beta_{N+1}}\delta^{\alpha_{N+1}}_{\alpha_1}. \quad (4)$$

Acting on the VBS state with the spin operators, we find that $S^a_0S^b_r$ breaks the string of valence bonds on one of the two links adjacent to site 0 and on one of the two links adjacent to site r, producing a product of two VBS states with the spin indices contracted with two Pauli matrices. Thus, the correlation function is determined by (4). We find, for an infinite chain,

$$\langle S^a_0S^b_r\rangle=\delta^{ab}(-1)^r\tfrac{4}{3}3^{-r}\text{ (for all } r>0).$$

Thus, the correlation function decays exponentially with correlation length $1/\ln 3\approx 0.9$.

Our solvable Hamiltonian of (1) is a special case of the general bilinear-biquadratic Hamiltonian

$$H=\textstyle\sum_i[\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\beta(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2],$$

with $\beta=-\frac{1}{3}$. The model with $\beta=1$ has been solved by the Bethe *Ansatz* method.[9] It has a unique ground state with *no* gap and appears to have *power-law* decay by standard field-theory arguments. We expect that $\beta=1$ is a critical point separating the VBS and dimerized phases (for $\beta<1$, and $\beta>1$, respectively). Translational symmetry is broken in one phase, but not the other. Exponential decay and a gap hold in both. A critical theory of this phase transition is given by Affleck[10] and Affleck and Haldane.[10] This picture is supported by finite-chain calculations.[11] For a *finite* even chain in the dimerized phase there is a unique ground state which is the symmetric combination of the two dimerized states. There is also an exponentially low-lying momentum-π singlet state which is the antisymmetric combination. For a finite odd chain, the ground state has spin 1 since there is one unpaired spin. We gave Hamiltonians above which had the simple dimerized ground states of Fig. 3. We can support this phase diagram by using the simple VBS and dimerized states as trial ground states for arbitrary β. The expectation of H (per link) in the VBS, dimerized, and Néel states is $(-\frac{4}{3}-2\beta)$, $(-1-8\beta/3)$, and $(-1-2\beta)$, respectively. Thus, the Néel state never has lowest energy while the VBS state is lowest for $\beta<\frac{1}{2}$, and the dimerized state for $\beta>\frac{1}{2}$. Of course, improving these variational VBS and dimerized states would change the estimated critical value of β.

For the realistic Hamiltonian with $\beta=0$, the energies are $-\frac{4}{3}$, -1, and -1. The exact value, obtained from finite-size extrapolation[12] is about -1.40. Since the VBS state is only higher in energy by about 0.07, it appears to be a good variational ground state. Perhaps more importantly, it provides a simple, intuitive picture of the nondegenerate massive phase.

A similar picture of the β dependence of the ground state is obtained from the large-n limit.[7] An SU(n) generalization of the bilinear spin-1 chain is obtained by letting the indices α run over $1,2,3,\ldots,n$. For the bilinear Hamiltonian, the VBS and dimerized states discussed above are both ground states in the large-n limit.[7] This is so because in that limit, H simply counts the number of nearest-neighbor valence bonds. The biquadratic term, in the large-n limit simply counts the number of nearest-neighbor *double* valence bonds.[6] Thus, the ground state is the VBS state for $\beta>0$, and the dimerized state for $\beta<0$. A first-order phase transition occurs at $\beta=0$. For the ordinary SU(2) case we expect the transition to be second order.[10]

A difference between integer and half-odd-integer spin chains, first predicted by Haldane,[1] emerges from the set of simple valence-bond states, as was observed earlier, in the context of the large-n limit.[7] While integer-spin chains can be in dimerized or VBS states, half-odd-

integer spin chains are necessarily at least partially dimerized. Of course, if the Hamiltonian is modified, the valence bonds could "resonate"[3] and the broken translational symmetry could then be restored. If this happens, leading to a unique ground state, the rigorous results of Affleck and Lieb[13] prove that there is a vanishing gap for half-odd-integer s. On the other hand, integer-spin chains *can* have ground states of unbroken symmetry with a gap, as our example proves. Thus, we have rigorously established that there is a difference between integer and half-odd-integer spin chains.

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Valence Bond Ground States in Isotropic Quantum Antiferromagnets

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Abstract. Haldane predicted that the isotropic quantum Heisenberg spin chain is in a "massive" phase if the spin is integral. The first rigorous example of an isotropic model in such a phase is presented. The Hamiltonian has an exact $SO(3)$ symmetry and is translationally invariant, but we prove the model has a unique ground state, a gap in the spectrum of the Hamiltonian immediately above the ground state and exponential decay of the correlation functions in the ground state. Models in two and higher dimension which are expected to have the same properties are also presented. For these models we construct an exact ground state, and for some of them we prove that the two-point function decays exponentially in this ground state. In all these models exact ground states are constructed by using valence bonds.

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1. Introduction

The ground state properties of quantum antiferromagnets not only have important physical consequences, they also contain some fascinating surprises. In one dimension the spin 1/2 Heisenberg antiferromagnet can be solved by the Bethe ansatz [11]. The correlation functions have power law decay and there exist local excitations with arbitrarily low energy, i.e., there is no gap in the spectrum immediately above the ground state energy. One might expect similar behavior in any one-dimensional isotropic quantum antiferromagnet. Haldane, however, argued that if the spin is integer then the one-dimensional Heisenberg antiferromagnet has completely different properties [23–25]. He concluded the ground state correlation functions have exponential decay and there is a gap in the spectrum above the ground state energy. There is both experimental and numerical support for these conclusions [12, 16, 36, 37 and references therein].

At first the existence of a gap in the spectrum and exponentially decaying correlation functions is surprising in a model with a continuous symmetry. However, there exist fairly simple models like the Majumdar-Ghosh model [31, 32] which have a translationally invariant Hamiltonian with a continuous symmetry, but have a gap and exponentially (or faster) decaying correlation functions. (Until now there was no proof that this model has a gap, but the proof is supplied in this paper.) In these models, however, the ground state is degenerate and breaks the translational symmetry while the usual Heisenberg antiferromagnet presumably has a unique ground state. The possibility of a quantum antiferromagnet with a continuous symmetry, exponentially decaying correlation functions, a gap *and* a unique ground state was quite unexpected. In this paper we provide the first rigorous example of a model with all these properties. The model is the one-dimensional spin chain with Hamiltonian

$$H = \sum_i [\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \tfrac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2]. \tag{1.1}$$

We prove this model has a unique infinite volume ground state, the correlation functions decay exponentially in this ground state, and there is a gap in the spectrum immediately above the ground state energy. It has been shown rigorously that models like (1.1) do not exhibit such behavior if the spin is half-integral [5].

In two or more dimensions one generally expects the ground states of quantum antiferromagnets to have Néel order. There is a Goldstone theorem for quantum spin systems which applies to a general class of isotropic Hamiltonians (which includes the usual Heisenberg Hamiltonian and the Hamiltonians we will consider in this paper) [44–46]. It states that *if there is Néel order then there is no gap.* The existence of Néel order in the ground state can be proven [21, 26] for the usual

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Heisenberg Hamiltonian on certain lattices if the spin is large enough, but there may be exceptions. Anderson has argued that the spin 1/2 model on a triangular lattice or a square lattice with a sufficiently strong next nearest neighbor coupling has a ground state without antiferromagnetic order [7]. His "resonating valence bond" (RVB) mechanism is the basis of a possible explanation of high T_c superconductors [8]. We provide an example of an isotropic antiferromagnet in two dimensions with spin 3/2 for which we can construct an exact ground state and prove that the two point function decays exponentially in this ground state. We expect that our model has a unique infinite volume ground state and a gap in its spectrum, but we cannot prove either of these conjectures. As in our one-dimensional model the Hamiltonian is isotropic, translationally invariant and can be written as a sum over nearest neighbor pairs i, j of polynomials in $\mathbf{S}_i \cdot \mathbf{S}_j$.

The construction of a ground state and proof of exponential decay of the two point function for our two-dimensional model can be adapted to any bipartite lattice with coordination number three. Since such lattices exist in any dimension greater than one, we expect that in any dimension greater than one there exist models with all the properties that Haldane predicts for the one-dimensional Heisenberg antiferromagnet with integer spin. *It should be emphasized that in dimensions greater than one it is not necessary that the spin be integral for this to happen. The relevant criterion appears to involve the lattice type (especially the coordination number), the spin and the dimension.*

Our one-dimensional model (1.1) is a special case of the Hamiltonian

$$H = \sum_i [\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2]. \tag{1.2}$$

The model with $\beta = 0$ is, of course, the standard Heisenberg model which is believed to have a unique massive ground state according to Haldane. We now know rigorously that such a unique massive ground state exists for $\beta = -1/3$. The model with $\beta = 1$, however, has been solved by the Bethe ansatz method [9, 10, 28, 29, 42]. It has a unique ground state with no energy gap, and appears to have power law decay of the correlation functions by standard field theory arguments. We expect that the model (1.2) has a unique massive ground state for $-1 < \beta < 1$ and undergoes a phase transition at $\beta = 1$ to a dimerized phase with two ground states and a gap for $\beta > 1$. At $\beta = -1$ the model has an exact $SU(3)$ symmetry and is very likely massless [3]. For more details and support for this picture we refer the reader to [1] and Sect. 4.4. Finite chain calculations supporting this picture may be found in [13, 20, 34, 41]. A critical theory for the phase transition at $\beta = 1$ based on the nonabelian bosonization method is given in [3, 4].

The possibility of an isotropic model with a unique massive ground state may be understood as follows. For a quantum antiferromagnet the quantum fluctuations always provide some "entropy," even in the ground state. Thus the ground state of a quantum antiferromagnet is like a classical model at some finite temperature. If this classical model is in a high temperature phase then the ground state of the quantum model will be unique and have a finite correlation length, i.e., a mass.

The key to all our models is the idea of a valence bond. Given two spin 1/2's, a valence bond is formed by putting them in the singlet state $\uparrow\downarrow - \downarrow\uparrow$. Now consider

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the spin 1 chain. Each spin 1 can be regarded as the symmetric part of the product of two spin 1/2's. We construct a state with a valence bond between each pair of adjacent sites i and $i+1$ by forming a singlet out of one of the spin 1/2's at site i and one at site $i+1$. After doing this we must symmetrize the two spin 1/2's at each site in order to restore spin 1 at each site. This state can be represented diagramatically as in Fig. 2.1. We call the resulting state a valence bond solid (VBS) state since the valence bond structure is identical to the underlying lattice. We will show in Sect. 2 that this state is a ground state of (1.1). This state was first introduced, to the best of our knowledge, in the discussion of the large n limit of $SU(n)$ chains [2]. Valence bonds have been used before to construct exact ground states [17, 18, 27, 38]. In these previous models, however, the ground states are at least doubly degenerate. Furthermore, these ground states can be written as a single tensor product of states, each of which only involves a few lattice sites. The VBS state cannot be written as such a tensor product.

Such VBS states can be constructed whenever the spin s equals 1/2 of the coordination number, z, of the lattice. A generalized VBS state can be constructed whenever s is an integer multiple of $z/2$ (see Sect. 6 for details). Hamiltonians for which these states are ground states can also be constructed. In one dimension the VBS states can be constructed if and only if the spin is integral. Thus these solvable models provide a qualitative explanation of why integer and half-integer spin chains should have such radically different behavior [2].

In two or more dimensions there are many VBS states because of the freedom at the boundary. We conjecture that if the coordination number z and dimension d are small enough then in the infinite volume limit there is a unique ground state and this state has exponentially decaying correlation functions and a gap. If z and d are large then we conjecture there is Néel order, no gap and infinitely many infinite volume ground states.

While we have no rigorous results on the nonzero temperature behavior of these models in two and more dimensions it is interesting to speculate on what happens. If there is a unique ground state and a gap above the energy of this ground state, then one would expect that for any temperature there is a unique Gibbs state and the correlation length remains bounded as the temperature goes to zero. In other words, it appears that in any dimension there exist isotropic quantum antiferromagnets which do not have a phase transition even at zero temperature.

The organization of the paper is as follows. Section 2 is devoted to the one-dimensional model (1.1). The exact ground state is constructed in detail and the two point function is calculated in this ground state. The existence of a gap, the uniqueness of the ground state and the exponential decay of all truncated correlation functions is proven. Our spin 3/2 model on a two-dimensional hexagonal lattice is defined and studied in Sect. 3. A ground state is constructed, and we prove that with periodic boundary conditions the two point function of the ground state has exponential decay. In Sect. 4 we construct the VBS state for a general lattice and speculate on how its properties depend on the dimension and lattice type. For the VBS state on the Cayley tree we show there is Néel order if the coordination number of the lattice exceeds four, but no Néel order when the coordination number equals three. We also discuss some $SU(n)$ models for which

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we can find exact ground states which are generalizations of the VBS state, and develop a random loop representation for these models. The Majumdar-Ghosh model is considered in Sect. 5. This model is known to have two ground states. We prove that these are the only two ground states in the infinite volume limit, and that there is a gap. In Sect. 6 we briefly discuss various generalizations of our models and the Majumdar-Ghosh model. In Appendix A we sketch how the standard technique of Gaussian domination shows that there is Néel order in the ground state of the usual Heisenberg antiferromagnet on the two-dimensional hexagonal lattice if the spin is at least 3/2.

The various sections of this paper are almost independent, so it should be possible to read any one section after a quick look at the preceding sections. Most of the results in this paper were announced in [1].

2. The One-Dimensional Model (1.1)

2.1. The Ground State

We define our one-dimensional system, and describe its exact ground states in some detail in this subsection. The calculation of the ground state correlation functions, the proof of the existence of an energy gap, and the proof of the uniqueness of the ground state will be given in the following subsections.

We denote sites in our one-dimensional lattice by i and denote the spin operator for spin $s=1$ at site i by $\mathbf{S}_i=(S^1{}_i, S^2{}_i, S^3{}_i)$. The restriction of a state to two adjacent sites i and $i+1$ can have spin 0, 1 or 2. We denote the orthogonal projection onto states with spin 2 by $P_2(\mathbf{S}_i+\mathbf{S}_{i+1})$. We can express this projection in terms of the spin operators as follows.

$$P_2(\mathbf{S}_i+\mathbf{S}_{i+1})=\mathbf{S}_i\cdot\mathbf{S}_{i+1}/2+(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2/6+1/3\,. \tag{2.1}$$

The Hamiltonian is the sum over i of these projections.

$$H=\sum_i H_i \quad \text{with} \quad H_i=P_2(S_i+S_{i+1})\,. \tag{2.2}$$

Obviously $H\geqq 0$, so if we could find a state Ω with $H_i\Omega=0$ for all i then Ω would be a ground state. Naively, one might not expect such a state to exist, but we will show that in fact it does.

To describe the exact ground states of the above Hamiltonian, we will introduce a special basis for the state space. First, consider the state space for a single spin 1/2. Let ψ_1, ψ_2 denote the eigenstates of S^3 with eigenvalues 1/2 and $-1/2$. The state space for spin 1 may be formed by taking the symmetric part of the tensor product of two spin 1/2 spaces. Thus an orthogonal basis is $\psi_{11}, \psi_{12}=\psi_{21}, \psi_{22}$, where

$$\psi_{\alpha\beta}=[\psi_\alpha\otimes\psi_\beta+\psi_\beta\otimes\psi_\alpha]/\sqrt{2}\,. \tag{2.3}$$

We emphasize that in this notation $\psi_{\alpha\beta}$ and $\psi_{\beta\alpha}$ denote the same state. These states do not all have norm 1. Their norms and overlaps are

$$(\psi_{\alpha\beta},\psi_{\gamma\delta})=\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}\,. \tag{2.4}$$

These states may be written in terms of a more standard basis for spin 1 as follows. Let $(+)$, (0), and $(-)$ denote the orthonormal basis for spin 1 consisting of eigenstates of S^3 with eigenvalues $+1$, 0, and -1, respectively. Then

$$\psi_{11}=\sqrt{2}(+), \quad \psi_{12}=\psi_{21}=(0), \quad \psi_{22}=\sqrt{2}(-). \tag{2.5}$$

Equation (2.4) hides the $SU(2)$ invariance of the theory. To make the invariance more explicit we should raise the indices of the state $\psi_{\alpha\beta}$ in the left side of the inner product. We accomplish this by adopting the physicists' notation $\psi^{\dagger\alpha\beta}\cdot\psi_{\gamma\delta}$ for the inner product $(\psi_{\alpha\beta},\psi_{\gamma\delta})$. Then (2.4) becomes

$$\psi^{\dagger\alpha\beta}\cdot\psi_{\gamma\delta}=\delta^{\alpha}{}_{\gamma}\delta^{\beta}{}_{\delta}+\delta^{\alpha}{}_{\delta}\delta^{\beta}{}_{\gamma}. \tag{2.6}$$

Both $\delta_{\alpha\gamma}$ and $\delta^{\alpha}{}_{\gamma}$ equal 1 if $\alpha=\gamma$ and 0 otherwise.

There are four spin 1/2's associated with each bond on the chain. If two of these spin 1/2's are in a singlet state, i.e., a state with total spin 0, then the four spin 1/2's can only have total spin 0 or 1. For two spin 1/2's, a singlet pair is formed by contracting with an ε tensor, i.e., $\psi_{\alpha}\otimes\psi_{\beta}\varepsilon^{\alpha\beta}$ is a singlet. ($\varepsilon^{\alpha\beta}$ is the antisymmetric tensor with $\varepsilon^{12}=1$.) In this expression and throughout the paper we adopt the convention that repeated upper and lower indices are summed. Given two spin 1's we can form $\Omega_{\alpha\beta}=\psi_{\alpha\gamma}\otimes\psi_{\delta\beta}\varepsilon^{\gamma\delta}$. Since two spin 1/2's are always in a singlet state in $\Omega_{\alpha\beta}$, $\Omega_{\alpha\beta}$ is a mixture of states with total spin 0 and 1. Hence $\Omega_{\alpha\beta}$ is a ground state (for two sites) of the projection onto spin 2.

It is now clear how we can form a ground state for a finite chain $\{1,2,\ldots,L\}$. For convenience we take L odd, but the definitions are essentially identical for even L. Let

$$\Omega_{\alpha\beta}=\psi_{\alpha\beta_1}\otimes\psi_{\alpha_2\beta_2}\otimes\ldots\otimes\psi_{\alpha_L\beta}\ \varepsilon^{\beta_1\alpha_2}\varepsilon^{\beta_2\alpha_3}\ldots\varepsilon^{\beta_{L-1}\alpha_L}. \tag{2.7}$$

For any two adjacent sites i and $i+1$, there is a spin 1/2 at site i and a spin 1/2 at site $i+1$ which are contracted with an ε tensor to form a singlet. Thus when $\Omega_{\alpha\beta}$ is restricted to sites i and $i+1$, it has only spin 0 and 1. Hence $H_i\Omega_{\alpha\beta}=0$, so $\Omega_{\alpha\beta}$ is a ground state of H.

We can simplify our notation by introducing a raising and lowering convention for indices and a shorthand notation for the tensor products. For spin 1/2 states we define $\psi^{\alpha}=\varepsilon^{\alpha\beta}\psi_{\beta}$ with the convention that repeated indices are summed. A singlet pair of spin 1/2's is then formed by contracting an upper and lower index, i.e., $\psi_{\alpha}\otimes\psi^{\alpha}$. For a single spin 1 we define

$$\psi^{\alpha\beta}=\varepsilon^{\alpha\gamma}\varepsilon^{\beta\delta}\psi_{\gamma\delta}. \tag{2.8}$$

It is easily checked that

$$(\psi^{\alpha\beta},\psi^{\gamma\delta})=\psi^{\dagger}{}_{\alpha\beta}\cdot\psi^{\gamma\delta}=\delta^{\gamma}{}_{\alpha}\delta^{\delta}{}_{\beta}+\delta^{\gamma}{}_{\beta}\delta^{\delta}{}_{\alpha}. \tag{2.9}$$

For our chain of spin 1's we raise the indices on every other site and introduce the shorthand,

$$\psi_{\alpha_1\beta_1}{}^{\alpha_2\beta_2\ldots\alpha_{L-1}\beta_{L-1}}{}_{\alpha_L\beta_L}=\psi_{\alpha_1\beta_1}\otimes\psi^{\alpha_2\beta_2}\otimes\ldots\otimes\psi^{\alpha_{L-1}\beta_{L-1}}\otimes\psi_{\alpha_L\beta_L}. \tag{2.10}$$

Then our ground state (2.7) is compactly written as

$$\Omega_{\alpha\beta}=\psi_{\alpha\alpha_1}{}^{\alpha_1\alpha_2}{}_{\alpha_2\alpha_3}{}^{\ldots\alpha_{L-2}\alpha_{L-1}}{}_{\alpha_{L-1}\beta}. \tag{2.11}$$

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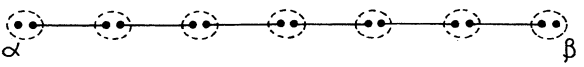

Fig. 2.1. The VBS state $\Omega_{\alpha\beta}$ on a finite chain. Each dot, line, and dotted circle represents a spin 1/2, a singlet pair, and the symmetrization of two spin 1/2's to create a spin 1

We can also define the periodic extension of H in (2.2) by adding $P_2(S_1+S_L)$ to H. This is also known as periodic boundary conditions. If L is odd then $\Omega=\Omega_{\alpha\beta}\varepsilon^{\alpha\beta}$ is a ground state. If L is even then $\Omega=\Omega_\alpha{}^\alpha$ is a ground state, where $\Omega_\alpha{}^\beta$ is the ground state given by the analog of (2.11) for even L.

There is a simple diagramatic representation of these VBS states. Each site in the chain is represented by two dots which represent the two spin 1/2's at that site. Each dot has a line coming out of it. Connecting two of these lines means that the two spin 1/2's are put in the singlet state. After forming these singlets we must symmetrize the two dots at each site. This symmetrization is represented by a dotted circle around the two dots. For an open chain there are free lines at each end of the chain corresponding to the indices α and β in $\Omega_{\alpha\beta}$. The resulting diagram for the ground state of an open chain is shown in Fig. 2.1.

We refer to these $\Omega_{\alpha\beta}$ and their (unique) infinite volume limit as *Valence-Bond Solid* (VBS) ground states. This terminology comes from the observation that, in these states, the valence bond (or singlet pair) structure exactly mimics the bond structure of the basic lattice. In Sects. 3, 4, and 6 we will discuss generalizations of VBS states to other lattices.

The VBS ground states appear very simple and natural in the present basis, but these states are not as trivial as they may appear. In particular, these states cannot be written as a single tensor product of a state at each site. To emphasize the richness of these states we will express them in terms of the usual $\{(+),(0),(-)\}$ basis of S^3 eigenstates at each site. The basis vectors for the chain are labelled by strings of 0's, +'s, and −'s. We denote such strings by A and the corresponding state by ψ_A. The coefficient of ψ_A in the ground state $\Omega_{\alpha\beta}$ will be denoted by $\Omega_{\alpha\beta}(A)$, so $\Omega_{\alpha\beta}=\sum_A \Omega_{\alpha\beta}(A)\psi_A$.

The coefficient $\Omega_{\alpha\beta}(A)$ is zero unless A is of a special form which depends on α and β. The rules are as follows:

$\alpha=1$, $\beta=2$: A must contain the same number of +'s and −'s. The first nonzero character in A must be a +, and thereafter the nonzero characters must alternate between − and +.

$\alpha=2$, $\beta=1$: Same as above with + and − reversed.

$\alpha=1$, $\beta=1$: A must contain one more + than −. The first nonzero character must be a +, and thereafter the nonzero characters must alternate between − and +.

$\alpha=2$, $\beta=2$: Same as above with + and − reversed.

An example of an A in the $\alpha=1$, $\beta=2$ class is $0+00-+0-0+000-$.

These four classes are disjoint with one exception; the string containing all 0's belongs to both the $\alpha=1$, $\beta=2$ class and the $\alpha=2$, $\beta=1$ class. Note that for any

choice of α and β, $\Omega_{\alpha\beta}(A)=0$ if A contains two $+$'s separated only by 0's or two $-$'s separated only by 0's.

We will give an explicit formula for $\Omega_{12}(A)$ and leave the other cases to the reader. Let A be a configuration in the class $\alpha=1$, $\beta=2$. Let k be the number of pairs of $+$ and $-$. Let m be the number of odd sites at which there is a $+$ or a $-$. Then

$$\Omega_{12}(A)=(-1)^m 2^k. \tag{2.12}$$

To show that this is a ground state, consider two adjacent sites i and $i+1$. It suffices to show that Ω_{12} is orthogonal to any state which has spin 2 on the pair of sites i and $i+1$. A basis for these spin 2 states is

$$\begin{aligned} e_1&=(++),\\ e_2&=(+0)+(0+),\\ e_3&=2(00)+(+-)+(-+),\\ e_4&=(-0)+(0-),\\ e_5&=(--). \end{aligned}$$

Obviously, Ω_{12} is orthogonal to e_1 and e_5. To see that Ω_{12} is orthogonal to e_2, let A be a string with $+$ at site i and 0 at site $i+1$. Let A' be the same string except that sites i and $i+1$ are interchanged. This switch leaves k unchanged but changes m by 1. Thus Eq. (2.12) implies that $\Omega_{12}(A)=-\Omega_{12}(A')$. So Ω_{12} is orthogonal to e_2, and, by the same argument, to e_4. Finally, to see that Ω_{12} is orthogonal to e_3, let A be a configuration with 0's at i and $i+1$. Let A_1 and A_2 be the two configurations obtained by replacing the two 0's by $-+$ and $+-$, respectively. Exactly one of A_1 and A_2 will have a nonzero coefficient. (Which one depends on α and β and on what A looks like off of sites i and $i+1$.) Assume A_1 has the nonzero coefficient. Then Eq. (2.12) yields $\Omega_{12}(A_1)=-2\Omega_{12}(A)$. It follows that Ω_{12} is orthogonal to e_3. Thus Eq. (2.12) defines a ground state.

Remarks. 1. For a finite chain with open boundary conditions we have found four ground states. In Sect. 2.2 we will calculate the norms and overlaps of these four states (2.14). It follows immediately from this calculation that the four ground states are nonzero and linearly independent. In Lemma 2.8 of Sect. 2.4 we will prove that they are the only finite volume ground states. Hence the open chain has a fourfold degenerate ground state. The total spin commutes with the Hamiltonian, so our four ground states must either consist of a triplet of spin 1 states and one spin 0 state or of four spin 0 states. The states $\Omega_{12}, \Omega_{21}, \Omega_{11}, \Omega_{22}$ have total S^3 equal to 0, 0, $+1$, -1, respectively. Hence we must have three spin 1 states (Ω_{11}, Ω_{22}, and a linear combination of Ω_{12} and Ω_{21}) and one spin 0 state (another linear combination of Ω_{12} and Ω_{21}). It is worth remarking that in the usual Heisenberg antiferromagnet the ground state for any L with open boundary conditions is always nondegenerate and has total spin 0 [30].

2. We can use Remark 1 to show that the periodic chain has a unique ground state. Suppose the periodic chain has a ground state with total spin 1. Then we can find a ground state for the periodic chain with total S^3 equal to $+1$. Any ground

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state for the periodic chain is also a ground state for the open chain, so this ground state must be a multiple of Ω_{11}. From the description of Ω_{11} in terms of 0's, +'s, and −'s, we see that Ω_{11} contains configurations with +'s at both sites 1 and L. Such a configuration, however, has spin 2 when restricted to sites 1 and L, and so is not a ground state for the periodic chain. This contradiction shows that the periodic chain only has ground states with total spin 0. The open chain has only one such ground state, so the periodic chain has a unique ground state.

3. In Sect. 2.4 we will show that the four ground states all yield the same state in the infinite volume limit and that the resulting infinite volume state is the only infinite volume ground state. In particular, the infinite volume limit constructed using periodic boundary conditions equals the infinite volume limit constructed using open boundary conditions.

2.2. The Ground State Two-Point Correlation Function

In this subsection we will calculate the two point correlation function for the ground state. By Remark 3 above, we need only perform the calculation for a particular choice of boundary conditions. We will use periodic boundary conditions. We will show that

$$\omega(S^a{}_0 S^b{}_r) = \delta^{ab}(-1)^r(4/3)3^{-r}, \tag{2.13}$$

where $\omega(S^a{}_0 S^b{}_r)$ denotes the limit as $L \to \infty$ of the expectation of $S^a{}_0 S^b{}_r$ in the ground state of the chain with L sites and periodic boundary conditions.

We begin by calculating the normalization of the ground state for an open chain of L sites. For later use we will actually calculate the inner product of any two of our four ground states. Since the notation depends on whether L is even or odd we assume that L is even. The basic formulae needed for this calculation are Eqs. (2.6) and (2.9). The calculation may be done in a diagramatic fashion using the diagrams introduced in Fig. 2.1.

We draw the state Ω twice, but label the two drawings as Ω and $\Omega^\dagger$ as shown in Fig. 2.2a. At each site the inner product is, according to (2.6) or (2.9), a sum of two terms. We represent them by Fig. 2.2b. Inserting Fig. 2.2b at each site in Fig. 2.2a gives a sum of 2^L diagrams. For example, with two sites the inner product is given by Fig. 2.2c. Each loop represents the trace of a product of δ tensors and so gives a factor of $\delta^\alpha{}_\alpha = 2$. Thus Fig. 2.2c yields

$$\begin{aligned}\Omega^{\dagger\alpha}{}_\beta \cdot \Omega_\gamma{}^\delta &= 2\delta^\alpha{}_\gamma \delta^\delta{}_\beta + \delta^\alpha{}_\gamma \delta^\delta{}_\beta + \delta^\alpha{}_\gamma \delta^\delta{}_\beta + \delta^\alpha{}_\beta \delta^\delta{}_\gamma \\ &= 4\delta^\alpha{}_\gamma \delta^\delta{}_\beta + \delta^\alpha{}_\beta \delta^\delta{}_\gamma .\end{aligned}$$

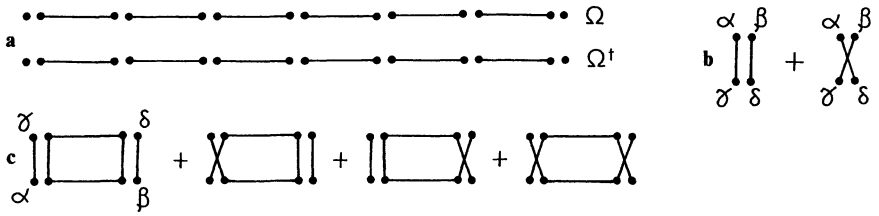

Fig. 2.2a–b. Inserting **b** into each site in **a** gives the overlap $\Omega^\dagger \cdot \Omega$. **c** The case with two sites

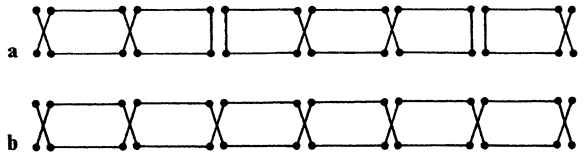

Fig. 2.3. Diagrams which appear in the overlap calculation. **a** A typical one, and **b** the special one has no loops

For general even L all but one diagram consists of an open line from α to γ, an open line from β to δ and some number of closed loops in between. A typical diagram is shown in Fig. 2.3a. All these diagrams give a contribution proportional to $\delta^{\alpha}{}_{\gamma}\delta^{\delta}{}_{\beta}$. The one other diagram consists of two lines stretching all the way across the lattice (Fig. 2.3b) and gives simply $\delta^{\alpha}{}_{\beta}\delta^{\delta}{}_{\gamma}$. Thus we need to perform the sum over all loop diagrams. For each loop we get a factor of 2 from $\delta^{\alpha}{}_{\alpha}=2$. The number of diagrams with m loops is the number of ways of choosing the $(m+1)$ points where the loops begin and end out of the L possible points, i.e., it is given by the binomial coefficient $\binom{L}{m+1}$. Thus the sum of all diagrams of this type is proportional to

$$\sum_{m=0}^{L-1}\binom{L}{m+1}2^m=[(2+1)^L-1]/2,$$

and so

$$\Omega^{\dagger\alpha}{}_{\beta}\cdot\Omega_{\gamma}{}^{\delta}=\delta^{\alpha}{}_{\gamma}\delta^{\delta}{}_{\beta}(3^L-1)/2+\delta^{\alpha}{}_{\beta}\delta^{\delta}{}_{\gamma}. \tag{2.14a}$$

If L is odd a similar computation yields

$$\Omega^{\dagger\alpha\beta}\cdot\Omega_{\gamma\delta}=\delta^{\alpha}{}_{\gamma}\delta^{\beta}{}_{\delta}(3^L-1)/2+\delta^{\alpha}{}_{\delta}\delta^{\beta}{}_{\gamma}. \tag{2.14b}$$

The normalization of the ground state with periodic boundary conditions

$$\Omega^{\dagger\beta}{}_{\beta}\cdot\Omega_{\alpha}{}^{\alpha}=3^L+3,$$

can be found by taking traces in (2.14) or by summing graphs on a circle.

Next we calculate the spin-spin correlation function for a chain with L sites and periodic boundary conditions. The spin operators acting on our basis for a single spin 1 give

$$S\psi_{\alpha\beta}=-(1/2)\sigma_{\alpha}{}^{\gamma}\psi_{\gamma\beta}-(1/2)\sigma_{\beta}{}^{\gamma}\psi_{\alpha\gamma}$$

on odd sites, or

$$S\psi^{\alpha\beta}=(1/2)\sigma^{\alpha}{}_{\gamma}\psi^{\gamma\beta}+(1/2)\sigma^{\beta}{}_{\gamma}\psi^{\alpha\gamma} \tag{2.15}$$

on even sites, where the $(\sigma^a)^{\alpha}{}_{\beta}$'s are the Pauli matrices and

$$\sigma^{\alpha}{}_{\beta}=\varepsilon^{\alpha\gamma}\varepsilon_{\beta\delta}\sigma_{\gamma}{}^{\delta}.$$

Thus acting with S_r on the periodic ground state, breaks either the link between sites $r-1$ and r or between r and $r+1$ and contracts the two dangling indices with

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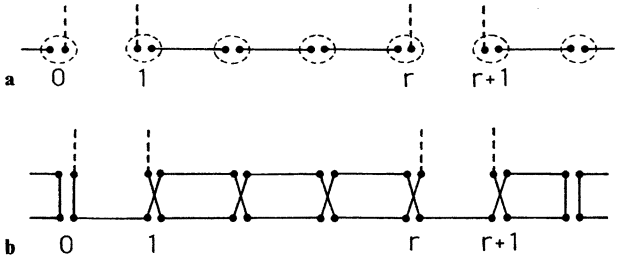

Fig. 2.4. **a** One of the four diagrams which represent the action of $S_0 \cdot S_r$ on Ω. **b** A typical diagram which gives a nonzero contribution to $\Omega^\dagger \cdot S_0 \cdot S_r \Omega$

$\pm(1/2)\sigma$ (for r even or odd). Acting with $S^a{}_0 S^b{}_r$ (we assume $r>2$) breaks the chain up into two open lines, one running from 0 or 1 to $r-1$ or r and the other running from r or $r+1$ to L or 0. One of these four cases is shown in Fig. 2.4a. The dangling indices near 0 are contracted with $(1/2)\sigma^a$ and those near r with $(-1)^r(1/2)\sigma^b$.

To obtain the correlation function we need to calculate the overlap of this state with the ground state. Again we represent the calculation by a sum of diagrams. There now must be two lines which end on the four dangling bonds, all others forming closed loops. These two lines can both stretch from 0 to $r(\pm 1)$ or one can start and end near 0, and the other start and end near r. There are far more diagrams of the latter type, however, they all give contributions proportional to $\delta^\alpha{}_\gamma(\sigma^a)_\alpha{}^\gamma \delta^\beta{}_\delta(\sigma^b)_\beta{}^\delta = \mathrm{Tr}\,\sigma^a \mathrm{Tr}\,\sigma^b = 0$. The former diagrams give contributions proportional to $(\sigma^a)_\alpha{}^\gamma \delta_\gamma{}^\beta (\sigma^b)_\beta{}^\delta \delta_\delta{}^\alpha = \mathrm{Tr}\,\sigma^a\sigma^b = 2\delta^{ab}$. The lines from 0 to r can run around the chain in either direction but for $L\to\infty$ with r fixed they must take the shorter path to contribute. Apart from these two lines there are one or more closed loops (many as $L\to\infty$) going around the chain the long way (see Fig. 2.4b). Summing over all these diagrams as before, being careful to sum over the four possible combinations of broken bonds and then dividing by the ground state normalization, we obtain (2.13).

2.3. The Energy Gap

We will prove that the Hamiltonian (2.2) has a gap between the ground state energy and the first excited state. In this subsection we begin by showing that for a finite chain of length L the gap is bounded away from zero as $L\to\infty$. In Sect. 2.4 we will show that the infinite volume system has a gap.

We use an open chain and assume that the four ground states we constructed in the previous section are the only ground states. We will prove they are the only ground states in Sect. 2.4. Bounding the gap away from zero uniformly in L is equivalent to the following theorem.

Theorem 2.1. *Consider the Hamiltonian*

$$H_{1,L} = \sum_{i=1}^{L-1} H_i . \tag{2.16}$$

There is a positive constant ε which does not depend on L such that

$$(\psi, H_{1,L}\psi) \geqq \varepsilon(\psi, \psi) \tag{2.17}$$

for all ψ which are orthogonal to the four ground states of $H_{1,L}$.

Proof. Our proof will take advantage of the following property of our model. If Ω is a ground state then for each i, $(\Omega, H_i\Omega)$ equals the lowest eigenvalue of H_i. Consequently, any ground state for $H_{1,n}$ is also a ground state for $H_{1,n-1}$.

Let Q_n be the orthogonal projection onto the subspace of states which are ground states for $H_{1,n}$, $n \leqq L$. Let $P_n = 1 - Q_n$. The previous paragraph implies $Q_n \geqq Q_{n+1}$, so $P_n \leqq P_{n+1}$. Inequality (2.17) is equivalent to $H_{1,L} \geqq \varepsilon P_L$. We write P_L as a sum of mutually orthogonal projections:

$$P_L = \sum_{n=l}^{L-1} (P_{n+1} - P_n) + P_l .$$

The integer l will be chosen later. It will be independent of L. (We assume, of course, that $L > l$.)

The idea of the proof is to bound $P_{n+1} - P_n = Q_n - Q_{n+1}$ by the terms H_i in the Hamiltonian with i near n. If we restrict $Q_n - Q_{n+1}$ to the first $n+1$ sites, then it is an 8-dimensional projection. (Q_n is 12-dimensional and Q_{n+1} is 4-dimensional.) Let $\varphi^i{}_{n+1}$, $i = 1, \ldots, 8$ be states on the first $n+1$ sites which are an orthonormal basis for the range of this projection. Each $\varphi^i{}_{n+1}$ is a ground state for $H_{1,n}$ and is orthogonal to any ground state for $H_{1,n+1}$.

Let $H_{n-l+1,n+1}$ be the Hamiltonian for sites $n-l+1$ to $n+1$, and let $Q_{n-l+1,n+1}$ be the orthogonal projection onto its ground states. Define

$$\psi^i{}_{n+1} = Q_{n-l+1,n+1}\varphi^i{}_{n+1} / \| Q_{n-l+1,n+1}\varphi^i{}_{n+1} \|$$

and define

$$\varepsilon(l) = \sup_n \max_i \| Q_{n-l+1,n+1}\varphi^i{}_{n+1} \|^2 .$$

We will reduce the proof to the following three lemmas.

Lemma 2.2. *Let e_{l+1} be the gap for $H_{1,l+1}$, i.e., the first nonzero eigenvalue of $H_{1,l+1}$. Then*

$$Q_n - Q_{n+1} \leqq 2\varepsilon(l) \sum_{i=1}^{8} P(\psi^i{}_{n+1}) + \frac{2}{e_{l+1}} H_{n-l+1,n+1} , \tag{2.18}$$

where $P(\psi^i{}_{n+1})$ is the orthogonal projection onto the states of the form $\psi^i{}_{n+1} \otimes \chi$ for any state χ on sites $n+2$ to L.

Lemma 2.3. *If $|m-n| \geqq l+1$ then for any i and j, $P(\psi^i{}_{n+1})$ is orthogonal to $P(\psi^j{}_{m+1})$, i.e., $P(\psi^i{}_{n+1})P(\psi^j{}_{m+1}) = 0$.*

Lemma 2.4. *There is a constant c such that for all l*

$$\varepsilon(l) \leqq c 3^{-l} . \tag{2.19}$$

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Assuming the three lemmas we complete the proof as follows. We will sum (2.18) from $n=l$ to $L-1$. Note that

$$\sum_{n=l}^{L-1}(Q_n-Q_{n+1})=Q_l-Q_L=P_L-P_l, \tag{2.20}$$

$$\sum_{n=l}^{L-1}H_{n-l+1,n+1}\leqq(l+1)H_{1,L}. \tag{2.21}$$

In the sum

$$\sum_{n=l}^{L-1}\sum_{i=1}^{8}P(\psi^i{}_{n+1}) \tag{2.22}$$

any two terms with $n=n_1$ and $n=n_2$ are orthogonal if $|n_1-n_2|>l$. Since any sum of mutually orthogonal projections is less than or equal to the identity operator, (2.22) is less than or equal to $8(l+1)$. Thus summing (2.18) yields

$$P_L-P_l\leqq 16(l+1)\varepsilon(l)+\frac{2(l+1)}{e_{l+1}}H_{1,L}.$$

Since e_l is the first positive eigenvalue of $H_{1,l}$, we trivially have

$$P_l\leqq\frac{1}{e_l}H_{1,l}\leqq\frac{1}{e_l}H_{1,L}.$$

Adding the above two inequalities implies

$$P_L\leqq 16(l+1)\varepsilon(l)+\left(\frac{2(l+1)}{e_{l+1}}+\frac{1}{e_l}\right)H_{1,L}.$$

Since P_L and $H_{1,L}$ can be simultaneously diagonalized, this implies inequality (2.17) provided $16(l+1)\varepsilon(l)<1$. By Lemma 2.4 we can make this quantity less than 1 by choosing l sufficiently large. Note that we have not assumed anything about how e_l depends on l. The only information we have used about e_l is that it is strictly positive. □

Proof of Lemma 2.2. In this proof we will abbreviate $Q_{n-l+1,n+1}$ by Q. Each operator in (2.18) acts as the identity on sites $n+2$ to L. Thus we may restrict our attention to sites 1 to $n+1$. For any state χ on sites 1 to $n+1$,

$$\begin{aligned}(\chi,P(\varphi^i{}_{n+1})\chi)&=|(\chi,\varphi^i{}_{n+1})|^2\\&=|(\chi,Q\varphi^i{}_{n+1}+(1-Q)\varphi^i{}_{n+1})|^2\\&\leqq 2|(\chi,Q\varphi^i{}_{n+1})|^2+2|(\chi,(1-Q)\varphi^i{}_{n+1})|^2,\end{aligned} \tag{2.23}$$

where we have used the Cauchy-Schwarz inequality to bound the cross terms. The first term equals

$$2\|Q\varphi^i{}_{n+1}\|^2(\chi,P(\psi^i{}_{n+1})\chi)\leqq 2\varepsilon(l)(\chi,P(\psi^i{}_{n+1})\chi),$$

since $\psi^i{}_{n+1}$ is defined as the unit vector proportional to $Q\varphi^i{}_{n+1}$. For the second term the orthonormality of the $\varphi^i{}_{n+1}$ implies

$$\sum_{i=1}^{8} |(\chi,(1-Q)\varphi^i{}_{n+1})|^2 = \sum_{i=1}^{8} |((1-Q)\chi,\varphi^i{}_{n+1})|^2 \leqq \|(1-Q)\chi\|^2 .$$

Thus summing (2.23) from $i=1$ to 8 we obtain

$$(\chi,(Q_n-Q_{n+1})\chi) = \sum_{i=1}^{8} (\chi,P(\varphi^i{}_{n+1})\chi) \leqq 2\varepsilon(l)\sum_{i=1}^{8}(\chi,P(\psi^i{}_{n+1})\chi)+2\|(1-Q)\chi\|^2 .$$

But $\|(1-Q)\chi\|^2=(\chi,(1-Q)\chi)$ and $1-Q\leqq H_{n-l+1,n+1}/e_{l+1}$. The lemma follows. □

Proof of Lemma 2.3. In this proof we abbreviate $Q_{n-l+1,n+1}$ and $Q_{m-l+1,m+1}$ by Q^n and Q^m. We can assume $m\geqq n+l+1$. To show the two projections are orthogonal, it suffices to show that the inner product $(Q^n\varphi^i{}_{n+1}\otimes\chi, Q^m\varphi^j{}_{m+1}\otimes\Theta)$ vanishes for any state χ on sites $n+2$ to L and any state Θ on sites $m+2$ to L. We should warn the reader that the two $\otimes$'s in this inner product mean different things. The first $\otimes$ indicates a tensor product between a state on sites 1 to $n+1$ and a state on sites $n+2$ to L. The second $\otimes$ indicates the same thing except that n is replaced by m.

Since Q^n and Q^m commute the inner product equals $(\varphi^i{}_{n+1}\otimes\chi, Q^mQ^n\varphi^j{}_{m+1}\otimes\Theta)$. But $\varphi^j{}_{m+1}$ is a ground state for $H_{1,m}$ and hence for $H_{n-l+1,n+1}$. So the inner product equals $(\varphi^i{}_{n+1}\otimes\chi, Q^m\varphi^j{}_{m+1}\otimes\Theta)$. Now $\varphi^j{}_{m+1}$ is a ground state for $H_{1,m}$ and so is a ground state for $H_{1,n+1}$. Since Q^m acts only on sites greater than $m-1$ and $m-1\geqq n+1$, $Q^m\varphi^j{}_{m+1}\otimes\Theta$ is also a ground state for $H_{1,n+1}$. But $\varphi^i{}_{n+1}$ is orthogonal to such states, so the inner product vanishes. □

Proof of Lemma 2.4. All of the states we will encounter in this proof will be linear combinations of the states shown diagramatically in Fig. 2.5. Our notation for this state depends on whether n and l are even or odd. For brevity we will only consider the case that n and l are both even. In this case the state in Fig. 2.5 is denoted by $\Omega_\alpha{}^\beta{}_\gamma{}^\delta{}_{\varepsilon\varrho}$. The argument in the other three cases is the same.

Let φ be one of the states $\varphi^i{}_{n+1}$. Then φ is a ground state of $H_{1,n}$ and so is a linear combination of the states $\Omega_\alpha{}^\beta{}_\beta{}^\delta{}_{\varepsilon\varrho}$, i.e.,

$$\varphi=\Omega_\alpha{}^\beta{}_\beta{}^\delta{}_{\varepsilon\varrho}A^\alpha{}_\delta{}^{\varepsilon\varrho}. \tag{2.24}$$

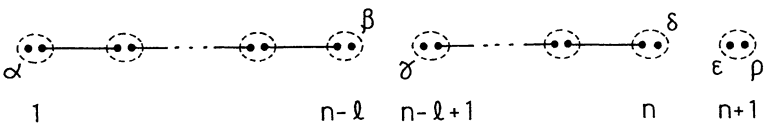

Fig. 2.5. The states $\Omega_\alpha{}^\beta{}_\gamma{}^\delta{}_{\varepsilon\varrho}$ which are used in the proof of the existence of a gap

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We can assume A is symmetric in ε and ϱ. Since $Q_{n+1}\varphi=0$, φ is orthogonal to the ground states of $H_{1,n+1}$, i.e., to the states $\Omega_{\mu\ \gamma\ \sigma\upsilon}^{\ \gamma\ \sigma}$. Using Eq. (2.14) this implies

$$\begin{aligned}0&=\Omega^{\dagger\mu\ \gamma\ \sigma\upsilon}_{\ \gamma\ \sigma}\cdot\varphi=\Omega^{\dagger\mu\ \gamma\ \sigma\upsilon}_{\ \gamma\ \sigma}\cdot\Omega_{\alpha\ \beta\ \varepsilon\varrho}^{\ \beta\ \delta}A^{\alpha\ \varepsilon\varrho}_{\ \delta}\\&=[\delta^{\mu}{}_{\alpha}\delta^{\delta}{}_{\sigma}(3^n-1)/2+\delta^{\delta}{}_{\alpha}\delta^{\mu}{}_{\sigma}][\delta^{\alpha}{}_{\varepsilon}\delta^{\upsilon}{}_{\varrho}+\delta^{\sigma}{}_{\varrho}\delta^{\upsilon}{}_{\varepsilon}]A^{\alpha\ \varepsilon\varrho}_{\ \delta}\\&=A^{\mu\ \delta\upsilon}_{\ \delta}(3^n-1)+2A^{\delta\ \mu\upsilon}_{\ \delta}.\end{aligned}$$

Thus

$$A^{\mu\ \delta\upsilon}_{\ \delta}=-2A^{\delta\ \mu\upsilon}_{\ \delta}/(3^n-1). \tag{2.25}$$

Thus whenever the second and third indices in $A^{\alpha\ \varepsilon\varrho}_{\ \delta}$ are contracted, the result is of order 3^{-n} compared with $A^{\alpha\ \varepsilon\varrho}_{\ \delta}$.

Our goal is to bound the square of the norm of $Q_{n-l+1,n+1}\varphi$. First, we show that this state is a linear combination of the states $\Omega_{\mu\ \sigma\ \gamma\omega}^{\ \upsilon\ \gamma}$. To do so we must show that $Q_{n-l+1,n+1}\varphi$ is a ground state of $H_{1,n-l}$ and of $H_{n-l+1,n+1}$. The latter case is trivial since $Q_{n-l+1,n+1}$ is the projection onto the ground states of $H_{n-l+1,n+1}$. The former case is also immediate since φ is a ground state of $H_{1,n}$ and so of $H_{1,n-l}$ and $Q_{n-l+1,n+1}$ commutes with $H_{1,n-l}$.

The number of states $\Omega_{\mu\ \sigma\ \gamma\omega}^{\ \upsilon\ \gamma}$ is independent of n and l, so the preceding paragraph implies that $\|Q_{n-l+1,n+1}\varphi\|^2=(Q_{n-l+1,n+1}\varphi,\varphi)$ is bounded by a constant times the sup over $\mu,\upsilon,\sigma,\omega$ of $|(\Omega_{\mu\ \sigma\ \gamma\omega}^{\ \upsilon\ \gamma},\varphi)|/\|\Omega_{\mu\ \sigma\ \gamma\omega}^{\ \upsilon\ \gamma}\|$. To compute this inner product we apply (2.14) twice, once for sites 1 to $n-l$ and once for sites $n-l+1$ to n. This yields

$$\begin{aligned}\Omega^{\dagger\mu\ \sigma\ \gamma\omega}_{\ \upsilon\ \gamma}\cdot\varphi&=\Omega^{\dagger\mu\ \sigma\ \gamma\omega}_{\ \upsilon\ \gamma}\cdot\Omega_{\alpha\ \beta\ \varepsilon\varrho}^{\ \beta\ \delta}A^{\alpha\ \varepsilon\varrho}_{\ \delta}\\&=[\delta^{\mu}{}_{\alpha}\delta^{\beta}{}_{\upsilon}(3^{n-l}-1)/2+\delta^{\beta}{}_{\alpha}\delta^{\mu}{}_{\upsilon}][\delta^{\sigma}{}_{\beta}\delta^{\delta}{}_{\gamma}(3^{l}-1)/2+\delta^{\sigma}{}_{\gamma}\delta^{\delta}{}_{\beta}]\\&\quad\times[\delta^{\gamma}{}_{\varepsilon}\delta^{\omega}{}_{\varrho}+\delta^{\gamma}{}_{\varrho}\delta^{\omega}{}_{\varepsilon}]A^{\alpha\ \varepsilon\varrho}_{\ \delta}\\&=A^{\mu\ \gamma\omega}_{\ \gamma}\delta^{\delta}{}_{\upsilon}(3^{n-l}-1)(3^{l}-1)/2+A^{\mu\ \sigma\omega}_{\ \upsilon}(3^{n-l}-1)\\&\quad+A^{\sigma\ \gamma\omega}_{\ \gamma}\delta^{\mu}{}_{\upsilon}(3^{l}-1)+2A^{\delta\ \sigma\omega}_{\ \delta}\delta^{\mu}{}_{\upsilon}.\end{aligned} \tag{2.26}$$

It is now clear how the proof works. In the first term the second and third indices of A are contracted. By (2.25) this gives us a factor of 3^{-n}. The other terms in the above sum are smaller than the first term by a factor of 3^{-l} or 3^{-n}. Since $n\geqq l$, the overlap in question is of order 3^{-l}.

To implement this intuition we need to consider the various normalizations. Recall that φ has norm 1 by definition. This implies, after some computation using Eqs. (2.14) and (2.24), that

$$1=A^{*\ \gamma}_{\mu\ \varepsilon\varrho}A^{\mu\ \varepsilon\varrho}_{\ \gamma}(3^n-1)/2+A^{*\ \delta}_{\delta\ \varepsilon\varrho}A^{\mu\ \varepsilon\varrho}_{\ \mu}.$$

($A^{*\ \gamma}_{\mu\ \varepsilon\varrho}$ denotes the complex conjugate of $A^{\mu\ \varepsilon\varrho}_{\ \gamma}$.) The second term in the right side is nonnegative and the first is just the sum over μ, γ, ε, and ϱ of $|A_{\mu\ \varepsilon\varrho}^{\ \gamma}|^2(3^n-1)/2$. Thus

$$|A_{\mu\ \varepsilon\varrho}^{\ \gamma}|^2\leqq 2(3^n-1)^{-1}. \tag{2.27}$$

The norm of $\Omega_{\mu\ \sigma\ \gamma\omega}^{\ \upsilon\ \gamma}$ can be computed using (2.14). The result is $3^{n+1}/4$ plus terms which are smaller by a factor of 3^{-n} or 3^{-l}. Combining this calculation with

(2.26) and (2.27) shows $|(\Omega_{\mu}{}^{\upsilon}{}_{\sigma}{}^{\gamma}{}_{\gamma\omega}, \varphi)|/\|\Omega_{\mu}{}^{\upsilon}{}_{\sigma}{}^{\gamma}{}_{\gamma\omega}\|$ is bounded by a constant times 3^{-l}. □

2.4. The Infinite Chain

In this subsection, we prove that the infinite volume system has a unique ground state, exponential decay of all truncated correlation functions in the ground state and a gap. We also prove that the finite volume ground states defined in Sect. 2.1 are the only ones. In this subsection instead of the finite chain $\{1, 2, \ldots, L\}$, we use the finite chain $\{-L, -L+1, \ldots, L\}$. The ground states for this finite chain are defined by analogy to (2.11) and denoted by $\Omega^{(L)}{}_{\alpha\beta}$. The natural way to construct an infinite volume ground state is to compute expectations in $\Omega^{(L)}{}_{\alpha\beta}$ and then let $L \to \infty$. Surprisingly, the result of this operation can be exactly expressed in terms of finite volume expectations as we will show in Lemma 2.6.

A *local observable, A*, is any polynomial in the spin operators for finitely many spins. (The identity operator I is a local observable.) If the spins involved in A involve only the sites $\{n, n+1, \ldots, n+m\}$ we say that the support of A is contained in $\{n, n+1, \ldots, n+m\}$. A *state* ϱ is a function on the local observables such that $\varrho(I) = 1$, $\varrho(\lambda A + \gamma B) = \lambda\varrho(A) + \gamma\varrho(B)$ for all $\lambda, \gamma \in C$ and $\varrho(A^* A) \geqq 0$ for all A.

Lemma 2.6. *Let A be a local observable. Then for any l such that the support of A is contained in $\{-l, -l+1, \ldots, l\}$,*

$$\lim_{L\to\infty} \frac{(\Omega^{(L)}{}_{\alpha\beta}, A\Omega^{(L)}{}_{\alpha\beta})}{(\Omega^{(L)}{}_{\alpha\beta}, \Omega^{(L)}{}_{\alpha\beta})} = \frac{\sum_{\varepsilon,\delta} (\Omega^{(l)}{}_{\varepsilon\delta}, A\Omega^{(l)}{}_{\varepsilon\delta})}{\sum_{\varepsilon,\delta} (\Omega^{(l)}{}_{\varepsilon\delta}, \Omega^{(l)}{}_{\varepsilon\delta})} \tag{2.28}$$

for any choice of α and β. (α and β are not summed over in this equation.) In particular, the limit in the left side of the equation exists and is independent of α and β. We denote this limit (which is a fortiori a state) by $\omega(A)$.

Proof. In this proof some repeated indices are not summed, so we will explicitly write out all summations. We can write $\Omega^{(L)}{}_{\alpha\beta}$ as

$$\Omega^{(L)}{}_{\alpha\beta} = \sum_{\gamma,\delta} \bar{\Omega}_{\alpha}{}^{\gamma} \Omega^{(l)}{}_{\gamma\delta} \tilde{\Omega}^{\delta}{}_{\beta}\,, \tag{2.29}$$

where $\bar{\Omega}_{\alpha}{}^{\gamma}$, $\Omega^{(l)}{}_{\gamma\delta}$, and $\tilde{\Omega}^{\delta}{}_{\beta}$ are ground states on $\{-L, \ldots, -l-1\}$, $\{-l, \ldots, l\}$, and $\{l+1, \ldots, L\}$, respectively. (We are assuming $L-l$ is even. If it is not, some indices must be raised or lowered.) This representation yields

$$(\Omega^{(L)}{}_{\alpha\beta}, A\Omega^{(L)}{}_{\alpha\beta}) = \sum_{\gamma,\delta,\varepsilon,\varrho} (\bar{\Omega}_{\alpha}{}^{\gamma}, \bar{\Omega}_{\alpha}{}^{\varepsilon})(\Omega^{(l)}{}_{\gamma\delta}, A\Omega^{(l)}{}_{\varepsilon\varrho})(\tilde{\Omega}^{\delta}{}_{\beta}, \tilde{\Omega}^{\varrho}{}_{\beta})\,.$$

By (2.14b),

$$(\bar{\Omega}_{\alpha}{}^{\gamma}, \bar{\Omega}_{\alpha}{}^{\varepsilon}) = \delta^{\varepsilon}{}_{\gamma}(3^{L-l}-1)/2 + \delta^{\gamma}{}_{\alpha}\delta^{\varepsilon}{}_{\alpha}\,,$$

$$(\tilde{\Omega}^{\delta}{}_{\beta}, \tilde{\Omega}^{\varrho}{}_{\beta}) = \delta^{\varrho}{}_{\delta}(3^{L-l}-1)/2 + \delta^{\beta}{}_{\delta}\delta^{\varrho}{}_{\beta}\,,$$

with no summation over α or β. Thus

$$(\Omega^{(L)}{}_{\alpha\beta}, A\Omega^{(L)}{}_{\alpha\beta}) = (3^{L-l}-1)^2/4 \sum_{\gamma,\delta} (\Omega^{(l)}{}_{\gamma\delta}, A\Omega^{(l)}{}_{\gamma\delta}) + \ldots\,, \tag{2.30}$$

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where the three terms represented by ... are all smaller by at least a factor of 3^{L-l}. The lemma now follows. □

Next we show that ω is the only infinite volume ground state.

Theorem 2.7. *Assume that a state ϱ on the infinite chain is ground state in the sense that ϱ satisfies $\varrho(H_i)=0$ for all i, where H_i is the local Hamiltonian defined in* (2.2). *Then the state ϱ equals the state ω defined in the previous lemma.*

Remark. Note that the definition of the ground state in the above theorem differs slightly from the "standard" definition in the mathematical physics literature. In the standard definition, the set of ground states G_0 is

$$G_0=\{\varrho \mid \varrho(A^*[H,A])\geqq 0 \text{ for an arbitrary local operator } A\},$$

while our ground state set G_1 is

$$G_1=\{\varrho \mid \varrho(H_i)=E_0 \text{ for all } i\},$$

where E_0 is the following ground state energy per site:

$$E_0=\inf_{\varrho}\lim_{N\to\infty}(1/N)\varrho\left(\sum_{i=-N/2}^{N/2}H_i\right).$$

Since some models have a state which belongs to G_0 but not to G_1 (e.g., the domain wall state in the Ising chain) we cannot expect these two definitions to be equivalent. Using the ergodic theorem [35], we can show that any translation invariant ϱ in G_0 also belongs to G_1. When E_0 happens to be the minimum eigenvalue of the local Hamiltonian H_i (as in our model), the standard property [14] of G_0 implies $G_1 \subset G_0$. In the present model, we expect that the two sets are identical. Another definition of the ground state, which is in many cases equivalent to G_0, can be found in [6].

The proof of the theorem is based on the lemma above and the following two lemmas.

Lemma 2.8 (Finite volume lemma). *Let φ be a state for the sites $-L$ to L which satisfies $H_i\varphi=0$ for $i=-L,\ldots,L-1$. Then φ can be written as*

$$\varphi=A^{\alpha\beta}\Omega^{(L)}{}_{\alpha\beta}, \tag{2.31}$$

where $A^{\alpha\beta}$ $(\alpha,\beta=1,2)$ are complex coefficients, and $\Omega^{(L)}{}_{\alpha\beta}$ are the finite volume ground states defined in (2.11).

Lemma 2.9. *Let A be an arbitrary local operator. Then*

$$\lim_{L\to\infty}\frac{(\Omega^{(L)}{}_{\alpha\beta}, A\Omega^{(L)}{}_{\gamma\delta})}{\|\Omega^{(L)}{}_{\alpha\beta}\|\,\|\Omega^{(L)}{}_{\gamma\delta}\|}=0 \quad \textit{(no sum over } \alpha,\ \beta,\ \gamma \textit{ or } \delta\textit{)}$$

for any α, β, γ, δ unless $\alpha=\gamma$, $\beta=\delta$.

Proof of Theorem 2.7. Assume that a state ϱ satisfies the condition. Let A be a local operator which acts on the spins in the interval $\{-L,\ldots,L\}$, and denote the restriction of ϱ to $\{-L,\ldots,L\}$ by ϱ_L. Since ϱ_L is a state on a finite system, ϱ_L has a

representation

$$\varrho_L(A)=\sum_a c_a(\varphi_a, A\varphi_a), \tag{2.32}$$

where $c_a \geqq 0$, $\sum_a c_a = 1$, and each φ_a is a normalized state which satisfies $H_i\varphi_a = 0$ for $i=-L,\ldots,L-1$. By Lemma 2.8 each φ_a is a linear combination of the finite volume ground states $\Omega^{(L)}{}_{\alpha\beta}$. Writing each φ_a in (2.32) as such a linear combination and using Lemmas 2.6 and 2.9, the theorem follows. □

Proof of Lemma 2.8. The proof proceeds by induction in the number of sites. For two sites the most general ground state (which must have no projection onto $s=2$) can be written

$$\Omega = \psi_{\alpha\beta}{}^{\beta\gamma} A^{\alpha}{}_{\gamma},$$

where $A^{\alpha}{}_{\gamma}$ is an arbitrary tensor. This can be checked by noting that there are four independent states of this type, corresponding to $s=0$ and $s=1$. Now let us consider a chain of three sites with open boundary conditions. Given a ground state Ω, since it has no projection onto $s=2$ for the first link, we can write it as

$$\Omega = \psi_{\alpha\beta}{}^{\beta\gamma}{}_{\delta\varepsilon} A^{\alpha}{}_{\gamma}{}^{\delta\varepsilon} \tag{2.33}$$

for some tensor $A^{\alpha}{}_{\gamma}{}^{\delta\varepsilon}$ which we may assume is symmetric in $\delta\varepsilon$ since $\psi_{\ldots\delta\varepsilon}$ is. Ω has no projection onto $s=2$ for the second link, so we may also write

$$\Omega = \psi_{\alpha\gamma}{}^{\delta\beta}{}_{\beta\varepsilon} B^{\alpha\gamma}{}_{\delta}{}^{\varepsilon}, \tag{2.34}$$

for some tensor $B^{\alpha\gamma}{}_{\delta}{}^{\varepsilon}$ which can be assumed to be symmetric in $\alpha\gamma$. Comparing these two forms of Ω, we see that $A^{\alpha}{}_{\gamma}{}^{\delta\varepsilon}=0$ unless $\gamma=\delta$ or $\gamma=\varepsilon$, since otherwise Ω would contain a term in which neither index on the second site was the same as either index on the third, and this would contradict (2.34). (This term arises by choosing $\beta=\gamma$.) Since $\psi_{\alpha\beta}{}^{\beta\gamma}{}_{\delta\varepsilon}$ is symmetric in $\delta\varepsilon$, (2.33) becomes

$$\Omega = \psi_{\alpha\beta}{}^{\beta 1}{}_{1\varepsilon} A^{\alpha}{}_{1}{}^{1\varepsilon} + \psi_{\alpha\beta}{}^{\beta 2}{}_{2\varepsilon} A^{\alpha}{}_{2}{}^{2\varepsilon}.$$

It only remains to prove that $A^{\alpha}{}_{1}{}^{1\varepsilon} = A^{\alpha}{}_{2}{}^{2\varepsilon}$. To prove this note that B can also be reduced in a similar way so that

$$\Omega = \psi_{\alpha 1}{}^{1\beta}{}_{\beta\varepsilon} B^{\alpha 1}{}_{1}{}^{\varepsilon} + \psi_{\alpha 2}{}^{2\beta}{}_{\beta\varepsilon} B^{\alpha 2}{}_{2}{}^{\varepsilon}.$$

Equating these two expressions we have

$$\begin{aligned}&\psi_{\alpha 1}{}^{11}{}_{1\varepsilon}(A^{\alpha}{}_{1}{}^{1\varepsilon} - B^{\alpha 1}{}_{1}{}^{\varepsilon}) + \psi_{\alpha 2}{}^{22}{}_{2\varepsilon}(A^{\alpha}{}_{2}{}^{2\varepsilon} - B^{\alpha 2}{}_{2}{}^{\varepsilon})\\ &\quad + \psi_{\alpha 1}{}^{12}{}_{2\varepsilon}(A^{\alpha}{}_{2}{}^{2\varepsilon} - B^{\alpha 1}{}_{1}{}^{\varepsilon}) + \psi_{\alpha 2}{}^{21}{}_{1\varepsilon}(A^{\alpha}{}_{1}{}^{1\varepsilon} - B^{\alpha 2}{}_{2}{}^{\varepsilon}) = 0.\end{aligned} \tag{2.35}$$

The coefficients of the first two terms must be zero, hence

$$A^{\alpha}{}_{1}{}^{1\varepsilon} = B^{\alpha 1}{}_{1}{}^{\varepsilon}, \quad A^{\alpha}{}_{2}{}^{2\varepsilon} = B^{\alpha 2}{}_{2}{}^{\varepsilon}. \tag{2.36}$$

The coefficient of the third term must be zero unless $\alpha=2$ and $\varepsilon=1$ in which case a contribution also arises from the fourth term,

$$A^{\alpha}{}_{2}{}^{2\varepsilon} = B^{\alpha 1}{}_{1}{}^{\varepsilon} \quad (\text{for } \alpha\varepsilon \neq 21). \tag{2.37}$$

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Finally, the coefficient of the fourth term must be zero unless $\alpha=1$ and $\varepsilon=2$.

$$A^{\alpha}{}_{1}{}^{1\varepsilon}=B^{\alpha 2}{}_{2}{}^{\varepsilon} \quad (\text{for } \alpha\varepsilon\neq 12). \tag{2.38}$$

Equations (2.36), (2.37), and (2.38) imply that

$$A^{\alpha}{}_{1}{}^{1\varepsilon}=A^{\alpha}{}_{2}{}^{2\varepsilon} \quad (\text{for all } \alpha,\varepsilon).$$

Thus we may write the most general ground state wave-function for three sites as

$$\Omega=\psi_{\alpha\beta}{}^{\beta\gamma}{}_{\gamma\varepsilon}C^{\alpha\varepsilon}$$

for some tensor $C^{\alpha\varepsilon}$.

To carry out the induction step define the following states on $N+1$ sites:

$$\Omega_{\alpha\beta}{}^{\gamma\delta}{}_{\varepsilon\varrho}=\psi_{\alpha\alpha_1}{}^{\alpha_1\alpha_2}{}_{\alpha_2\alpha_3\ldots\alpha\beta}{}^{\gamma\delta}{}_{\varepsilon\varrho}.$$

Let Ω be a ground state for $N+1$ sites. Then it is a ground state for N sites and so by induction

$$\Omega=\Omega_{\alpha\beta}{}^{\beta\delta}{}_{\varepsilon\varrho}A^{\alpha}{}_{\delta}{}^{\varepsilon\varrho}.$$

Since Ω has no projection onto spin 2 for sites N and $N+1$,

$$\Omega=\Omega_{\alpha\beta}{}^{\gamma\delta}{}_{\delta\varrho}B^{\alpha\beta}{}_{\gamma}{}^{\varrho}.$$

The argument for three sites can now be used to conclude

$$\Omega=\Omega_{\alpha\beta}{}^{\beta\delta}{}_{\delta\varrho}C^{\alpha\varrho}. \quad \square$$

Proof of Lemma 2.9. The technique used to prove Lemma 2.6, namely Eq. (2.29), can also be used to prove Lemma 2.9. The details are left to the reader. $\square$

Next we show that any truncated correlation function for the ground state has exponential decay.

Theorem 2.10. *Let A and B be local observables and let d be the distance between their supports. Then*

$$|\omega(AB)-\omega(A)\omega(B)|\leqq 3^{-(d-2)}\|A\|\,\|B\|.$$

Proof. For this proof we also write out any summations explicitly. Assume that the support of A is to the left of the support of B and let r be the right-most site in the support of A and $r+d$ the left-most site in the support of B. The argument is similar to that for Lemma 2.6. Choose L large enough that the supports of A and B are in $\{-L,\ldots,L\}$. Write $\Omega^{(L)}{}_{\alpha\beta}$ as

$$\Omega^{(L)}{}_{\alpha\beta}=\sum_{\gamma,\delta}\bar{\Omega}_{\alpha}{}^{\gamma}\Omega'{}_{\gamma\delta}\tilde{\Omega}^{\delta}{}_{\beta},$$

where $\bar{\Omega}_{\alpha}{}^{\gamma}$, $\Omega'{}_{\gamma\delta}$, and $\tilde{\Omega}^{\delta}{}_{\beta}$ are now ground states on $\{-L,\ldots,r\}$, $\{r+1,\ldots,r+d-1\}$, and $\{r+d,\ldots,L\}$, respectively.

By Lemma 2.6 we can compute $\omega(AB)$ by computing

$$\sum_{\alpha,\beta}(\Omega^{(L)}{}_{\alpha\beta},AB\Omega^{(L)}{}_{\alpha\beta})=\sum_{\alpha,\beta,\gamma,\delta,\varepsilon,\varrho}(\bar{\Omega}_{\alpha}{}^{\gamma},A\bar{\Omega}_{\alpha}{}^{\varepsilon})(\Omega'{}_{\gamma\delta},\Omega'{}_{\varepsilon\varrho})(\tilde{\Omega}^{\delta}{}_{\beta},B\tilde{\Omega}^{\varrho}{}_{\beta}).$$

Using (2.14) to compute $(\Omega'_{\gamma\delta}, \Omega'_{\varepsilon\varrho})$, we see this equals

$$=(3^{d-1}-1)/2 \sum_{\alpha,\gamma} (\bar{\Omega}_\alpha{}^\gamma, A\bar{\Omega}_\alpha{}^\gamma) \sum_{\beta,\delta} (\tilde{\Omega}^\delta{}_\beta, B\tilde{\Omega}^\delta{}_\beta)$$
$$+ \sum_{\alpha,\beta,\gamma,\varepsilon} (\bar{\Omega}_\alpha{}^\gamma, A\bar{\Omega}_\alpha{}^\varepsilon)(\tilde{\Omega}^\varepsilon{}_\beta, B\tilde{\Omega}^\gamma{}_\beta).$$

Using Lemma 2.6 again, the first term when normalized becomes $\omega(A)\omega(B)(1-3^{-(d-1)})$. The second term when normalized is easily bounded by a constant times $\|A\|\,\|B\|3^{-(d-1)}$. Keeping track of the constants yields the result stated in the theorem. □

Finally, we show that the infinite volume system has a gap. There are various definitions of the existence of a gap for the infinite volume system. We use the following one.

Definition 2.11. If ω is a ground state then ω has a gap ε if for every local observable A such that $\omega(A)=0$ we have

$$\omega(A^*[H,A]) \geqq \varepsilon\omega(A^*A).$$

Theorem 2.12. *The state ω defined in Lemma 2.6 has a gap.*

Proof. Let A be a local observable such that $\omega(A)=0$. Pick some α and β. By Lemma 2.6

$$\lim_{L\to\infty} \frac{(\Omega^{(L)}{}_{\alpha\beta}, A\Omega^{(L)}{}_{\alpha\beta})}{(\Omega^{(L)}{}_{\alpha\beta}, \Omega^{(L)}{}_{\alpha\beta})} = \omega(A) = 0.$$

Thus the overlap of $A\Omega^{(L)}{}_{\alpha\beta}$ with $\Omega^{(L)}{}_{\alpha\beta}$ is $o(1)$ with respect to the norms involved as $L\to\infty$. By Lemma 2.9, the overlap of $A\Omega^{(L)}{}_{\alpha\beta}$ with $\Omega^{(L)}{}_{\gamma\delta}$ is $o(1)$ with respect to the norms involved unless $\alpha=\gamma$ and $\beta=\delta$. Thus the norm of the projection of $A\Omega^{(L)}{}_{\alpha\beta}$ onto the subspace of ground states of the finite chain is $o(1)$ with respect to $\|A\Omega^{(L)}{}_{\alpha\beta}\|$. By Theorem 2.1 the finite chain has a gap ε, so

$$(\Omega^{(L)}{}_{\alpha\beta}, A^*[H,A]\Omega^{(L)}{}_{\alpha\beta}) \geqq (\varepsilon - o(1))(\Omega^{(L)}{}_{\alpha\beta}, A^*A\Omega^{(L)}{}_{\alpha\beta}).$$

The theorem follows. □

3. The Spin 3/2 Model on the Hexagonal Lattice

3.1. The Ground State

Here we describe our results on the Valence-Bond solid state on the two-dimensional hexagonal lattice. We show that the state, which is an exact ground state of a certain Hamiltonian, exhibits properties similar to those of the one-dimensional VBS state. We also present models in higher dimensions which have similar ground states. Though our rigorous results are less complete than those for the one-dimensional model, they provide the first concrete examples in two and higher dimensions of exact disordered ground states which appear to be unique.

In the present subsection, we describe the model and its exact ground state precisely. Let Λ be the set of sites in the finite hexagonal lattice with periodic boundary conditions. The set of bonds $\mathbb{B}$ consists of unordered pairs (i, j) of

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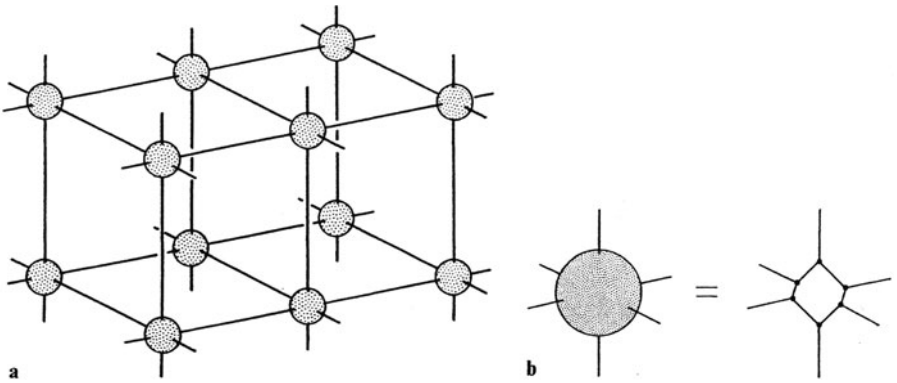

Fig. 3.1. **a** The cubic lattice with **b** decorated vertices is a three-dimensional bipartite lattice with coordination number three

adjacent sites i, j in Λ. Note that the hexagonal lattice is a bipartite lattice, i.e., it can be decomposed into two sublattices Λ_A and Λ_B with the properties that $\Lambda_A \cup \Lambda_B = \Lambda$, $\Lambda_A \cap \Lambda_B = \emptyset$, and for any $(i, j) \in \mathbb{B}$, either $i \in \Lambda_A$, $j \in \Lambda_B$ or $j \in \Lambda_A$, $i \in \Lambda_B$.

All the results in the present section can be generalized to *arbitrary* bipartite lattices with coordination number three. Among the examples of such lattices are the one-dimensional ladder lattice, the two-dimensional hexagonal lattice, and various lattices [43] with dimensions three or higher. An example of such a lattice in three dimensions is given in Fig. 3.1. We can modify this lattice so that all the bonds have unit length, and any pair of sites separated by unit length are connected by a bond. However, we note that such an example is primarily of theoretical interest and has little direct connection with physical experiments. The importance of these examples is that they show that isotropic antiferromagnets in dimensions greater than one may exhibit the same properties that Haldane predicted for the Heisenberg chain. (In Sect. 4, we discuss lattices with coordination numbers greater than three.)

Let us associate a spin operator $\mathbf{S}_i$ with spin $s = 3/2$ with site i. Then our Hamiltonian is

$$H = \sum_{(i,j) \in \mathbf{B}} P_3(\mathbf{S}_i + \mathbf{S}_j) = \sum_{(i,j) \in \mathbf{B}} H_{ij}, \tag{3.1}$$

where $P_3(\mathbf{S})$ is the orthogonal projection onto the states with $\mathbf{S}^2 = 3(3+1)$ (spin 3).

Note that our Hamiltonian describes antiferromagnetic pairwise interactions with perfect $SO(3)$ symmetry. To see that (3.1) has an antiferromagnetic character, observe that the energy is higher when the two neighboring spins add up to the maximum spin. This Hamiltonian is also equivalent to the following polynomial of the spin operators.

$$\sum_{(i,j) \in \mathbf{B}} [\mathbf{S}_i \cdot \mathbf{S}_j + \tfrac{116}{243}(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \tfrac{16}{243}(\mathbf{S}_i \cdot \mathbf{S}_j)^3]. \tag{3.1'}$$

To extend the VBS ground state to the hexagonal lattice, we think of spin 3/2 as the symmetric part of the product of three spin 1/2's. For a single site, our basis

consists of four vectors ψ_{111}, $\psi_{112}=\psi_{121}=\psi_{211}$, $\psi_{122}=\psi_{212}=\psi_{221}$, and ψ_{222} which are defined as

$$\psi_{\alpha_1\alpha_2\alpha_3}=\sum_{(\alpha_1,\alpha_2,\alpha_3)\to(\beta_1,\beta_2,\beta_3)}\psi_{\beta_1}\otimes\psi_{\beta_2}\otimes\psi_{\beta_3}/\sqrt{3!}\,. \tag{3.2}$$

Here $\{\psi_1=(+),\ \psi_2=(-)\}$ denotes the standard S^3 eigenstate basis for spin 1/2, and the summation runs over all the permutations of $(\alpha_1,\alpha_2,\alpha_3)$. The normalization condition for these vectors is

$$(\psi_{\alpha_1\alpha_2\alpha_3},\psi_{\beta_1\beta_2\beta_3})=\sum_{(\beta_1,\beta_2,\beta_3)\to(\gamma_1,\gamma_2,\gamma_3)}\delta_{\alpha_1\gamma_1}\delta_{\alpha_2\gamma_2}\delta_{\alpha_3\gamma_3}\,. \tag{3.3}$$

Therefore, our basis is related to the standard S^3 eigenstate basis for $s=3/2$ by the following.

$$(+3/2)=\psi_{111}/\sqrt{6},\quad (+1/2)=\psi_{112}/\sqrt{2},$$
$$(-1/2)=\psi_{122}/\sqrt{2},\quad (-3/2)=\psi_{222}/\sqrt{6}.$$

Again we use the following convention for raising indices

$$\psi^{\alpha_1\alpha_2\alpha_3}=\varepsilon^{\alpha_1\beta_1}\varepsilon^{\alpha_2\beta_2}\varepsilon^{\alpha_3\beta_3}\psi_{\beta_1\beta_2\beta_3}$$

and a summation convention for repeated upper and lower indices.

Let i_1, i_2, and i_3 be the three neighboring sites of a site i. We represent a state on site i as

$$\psi_{\alpha_{ii_1}\alpha_{ii_2}\alpha_{ii_3}}$$

if $i\in\Lambda_A$, and as

$$\psi^{\alpha_{ii_1}\alpha_{ii_2}\alpha_{ii_3}}$$

if $i\in\Lambda_B$. Then the VBS state on the hexagonal lattice is obtained by letting each pair of spin 1/2's on adjacent sites form a singlet pair.

$$\Omega_A=\bigotimes_{i\in\Lambda_A}\psi_{\alpha_{ii_1}\alpha_{ii_2}\alpha_{ii_3}}\bigotimes_{j\in\Lambda_B}\psi^{\alpha_{jj_1}\alpha_{jj_2}\alpha_{jj_3}}. \tag{3.4}$$

Note that for any $(i, j)\in\mathbb{B}$, both indices α_{ij} and α_{ji} appear exactly once in the above expression. Since one of them appears as an upper index, and the other appears as a lower index, we can sum over them by setting $\alpha_{ij}=\alpha_{ji}$. Then all the indices in (3.4) are contracted, and we get a single state Ω_A where the valence bond structure is identical to the bond structure of the lattice (Fig. 3.2).

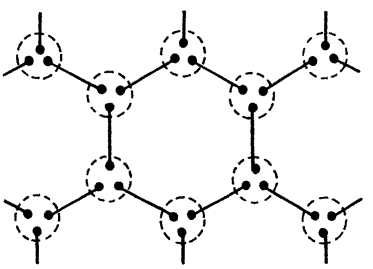

Fig. 3.2. The VBS state on the hexagonal lattice. Each dot, line, and dotted circle represents a spin 1/2, a singlet pair, and the symmetrization of three spin 1/2's to create a spin 3/2

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To see that the state Ω_Λ is actually an exact ground state of the Hamiltonian (3.1), note that the restriction of the state to an arbitrary pair of adjacent sites contains at least one singlet pair. Therefore, the total spin of these two sites is always 2, 1 or 0, which means $H_{ij}\Omega_\Lambda = 0$ for any $(i, j) \in \mathbb{B}$. Since 0 is the minimum eigenvalue of the local Hamiltonian H_{ij}, Ω_Λ is an exact ground state.

It is desirable to have an argument for the uniqueness of the infinite volume ground state (like Theorem 2.7) for the hexagonal lattice model (3.1). In fact, we expect the analog of Lemma 2.8 (finite volume lemma) to be valid for the general class of VBS systems (which is described in Sects. 4 and 6) including the present one. Moreover, our result on the exponential decay of the two point correlation function suggests that the analog of Lemma 2.6 is also valid in the present model (for a bipartite lattice with coordination number three). See note added in proof.

3.2. Properties of the Ground State

The main result of the present section is in the following theorem which establishes the exponential decay of the correlation function in the VBS state (3.4). The proof of the theorem will be presented in the next subsection.

Theorem 3.1. *The two point correlation function of the VBS state with periodic boundary conditions* (3.4)

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_\Lambda = \frac{(\Omega_\Lambda, \mathbf{S}_i \cdot \mathbf{S}_j \Omega_\Lambda)}{(\Omega_\Lambda, \Omega_\Lambda)} \tag{3.5}$$

satisfies the bound

$$0 \leqq (-1)^{i-j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_\Lambda \leqq C \exp(-|i-j|/\xi_0) \tag{3.6}$$

for any $i, j \in \Lambda$. Here C and ξ_0 are positive constants which are independent of the lattice size, $(-1)^{i-j} = 1$ or -1 according to whether i and j belong to the same sublattice or not, and $|i-j|$ denotes the graph theoretic distance (i.e., the minimum number of bonds needed to connect i and j.)

Note that ξ_0 in the theorem provides an upper bound for the actual correlation length. From our proof in the next subsection, we get $\xi_0 = \{\ln(2/\sqrt{6})\}^{-1} = 4.93\ldots$. For the hexagonal lattice, we may use the "exact but nonrigorous" value [33] of the entropy of self-avoiding random walks to get an improved upper bound $\xi_1 = 3.54\ldots$.

Let us describe some physical consequences of our theorem. Consider the following infinite volume limit of the VBS state Ω_Λ,

$$\omega(A) = \lim_{\Lambda \to \Lambda_\infty} \frac{(\Omega_\Lambda, A\Omega_\Lambda)}{(\Omega_\Lambda, \Omega_\Lambda)}. \tag{3.7}$$

Here Λ_∞ denotes the infinite hexagonal lattice. By symmetry

$$\omega(\mathbf{S}_i) = \lim_{\Lambda \to \Lambda_\infty} \langle \mathbf{S}_i \rangle_\Lambda = (0, 0, 0).$$

At the same time, since our upper bound (3.6) is uniform in Λ, the corresponding bound is also valid for the correlation function $\omega(\mathbf{S}_i \cdot \mathbf{S}_j)$ of infinite volume VBS state (3.7). This fact strongly suggests that ω is a *pure state.*

Therefore, we conjecture that ω is the unique infinite volume ground state of the Hamiltonian (3.1), and has no Néel ordering. It has been argued that ground states of two-dimensional antiferromagnets usually have Néel order. Though some examples of non Néel ordered exact ground states are known [27], they are infinitely degenerate and exhibit trivial ultra short range correlation functions (see also Sect. 6). As far as we know, the VBS states (3.4) are the first examples in two and higher dimensions of disordered exact ground state which are presumably unique. Note that the VBS state is qualitatively different from Anderson's disordered ground state (resonating valence-bond) on the triangular lattice [7]. However, it is interesting that valence bonds seem to play crucial roles in both cases.

The exponential fall-off of the correlation function also suggests the existence of an energy gap in the Hamiltonian (3.1). However, we do not know any way of proving (or disproving) this conjecture.

Finally, let us briefly discuss the relevance of our results and speculations to Hamiltonians other than (3.1). First of all the (conjectured) uniqueness of the ground state and the (conjectured) existence of an energy gap suggest that our hexagonal lattice VBS state is in some sense stable under a perturbation of the Hamiltonian. In particular, if we start from the Hamiltonian (3.1) and add some "small" perturbation, the resulting ground state is expected to have the same properties as the VBS state, i.e., exponentially decaying correlation functions, an energy gap, and no Néel order. We say that such a ground state is in the *VBS phase.* Then a natural question is whether a system with the most standard (and realistic) purely bilinear Heisenberg Hamiltonian

$$H = \sum_{(i,j)\in \mathbf{B}} \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.8}$$

is in the VBS phase or not. As we discuss in the appendix, the reflection positivity argument of [21, 26] is strong enough to prove the existence of Néel order in the ground state of an $s=3/2$ antiferromagnet on the hexagonal lattice with bilinear Hamiltonian (3.8). Thus as we change the Hamiltonian continuously from (3.1′) to (3.8), a (second order?) phase transition from the VBS phase to the Néel ordered phase takes place at a certain Hamiltonian. Moreover, it is also possible that the VBS phase is realized in Hamiltonians which are not at all close to (3.1). For example, a bilinear Hamiltonian with nonnearest neighbor couplings sufficiently large to destroy Néel order could be in the VBS phase.

3.3. Proof of Exponential Decay

The present subsection is devoted to the proof of Theorem 3.1. The starting point of our proof is the following *polymer representation* of the VBS state (3.4). Note that in (3.4), there is a one-to-one correspondence between the lattice bonds and the pairs of repeated upper and lower indices. Therefore, each term in (3.4) can be represented by assigning the values $\alpha_{ij}=1$ or 2 to every bond in the lattice. By

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denoting the set of bonds with $\alpha_{ij}=1$ by G, we can rewrite (3.4) as

$$\Omega_\Lambda = \sum_{G\subset \mathbf{B}} \Phi(\{n_k(G)\}_{k\in\Lambda}), \tag{3.9}$$

where G runs over all the subsets of the lattice bonds. $n_k(G)$ denotes the number of the bonds in G incident to a site k, and the basis states are given by

$$\Phi(\{n_k(G)\}_{k\in\Lambda}) = \bigotimes_{l\in\Lambda_A} \psi_{n_l(G)} \bigotimes_{m\in\Lambda_B} \psi^{n_m(G)}. \tag{3.10}$$

Here ψ_n (respectively, ψ^n) $(n=0,1,2)$ denotes the basis vector $\psi_{\alpha_1\alpha_2\alpha_3}$ (respectively, $\psi^{\alpha_1\alpha_2\alpha_3}$), where n of the three indices are 1.

Remark. The polymer representation (3.9) is also valid for the $s=1$ VBS state on the one dimensional chain where our basis is related to the standard S^3 eigenstate basis as

$$\psi_0=\psi^2=\sqrt{2}(+), \quad \psi_1=-\psi^1=(0), \quad \psi_2=\psi^0=\sqrt{2}(-).$$

Inserting this relation into (3.9) and rewriting each term in the standard basis, we get the representation of the $s=1$ VBS state presented at the end of Sect. 2.1.

Consider the norm $(\Omega_\Lambda, \Omega_\Lambda)$ of the VBS state (3.4). From (3.9) and the inner product formula (3.3), we easily find that

$$\begin{aligned}(\Omega_\Lambda, \Omega_\Lambda) &= \sum_{G',G\subset \mathbf{B}} (\Phi(\{n_k(G')\}_{k\in\Lambda}), \Phi(\{n_k(G)\}_{k\in\Lambda})) \\ &= \sum_{G',G\subset \mathbf{B}} \prod_{k\in\Lambda} \chi(n_k(G')=n_k(G)) n_k(G)!\,(3-n_k(G))!\,, \end{aligned} \tag{3.11}$$

where the characteristic function $\chi(A)$ is 1 if A is true, and 0 if A is false. It is useful to represent the above expression geometrically. For a given pair G', G, we draw a graph like Fig. 3.3a by putting a straight segment on each bond in G, and a wavy segment on each bond in G'. From (3.11), we find that a graph contributes to the norm $(\Omega_\Lambda, \Omega_\Lambda)$ if and only if for each site the number of straight segments incident to the site equals the number of wavy segments incident to the site.

Let $S^+=(S^1+iS^2)/2$ and $S^-=(S^1-iS^2)/2$ be the usual raising and lowering operators, respectively. It is easy to check that these operators acting on our basis give

$$S^+\psi_n=(3-n)\psi_{n+1}, \quad S^-\psi_n=n\psi_{n-1}. \tag{3.12}$$

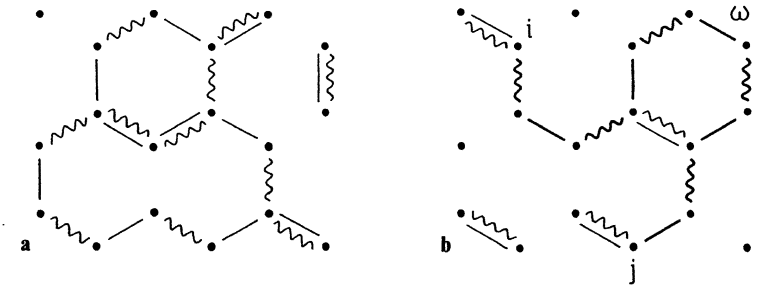

Fig. 3.3. **a** A graph which contributes to $(\Omega_\Lambda, \Omega_\Lambda)$. **b** A graph which contributes to $(\Omega_\Lambda, S^+_i S^-_j \Omega_\Lambda)$. The thicker lines represent the self-avoiding walk ω

Let i and j be sites in Λ_B. Then from (3.10) and (3.12), we find

$$S^+{}_i S^-{}_j \Phi(\{n_k(G)\}_{k\in\Lambda}) = (3-n_i(G))n_j(G)\Phi(\{n_k(G)+\delta_{k,i}-\delta_{k,j}\}_{k\in\Lambda}).$$

This formula and (3.9) imply the following expression for the unnormalized correlation function:

$$\begin{aligned}&(\Omega_\Lambda, S^+{}_i S^-{}_j \Omega_\Lambda)\\ &= \sum_{G',G\subset\mathbb{B}} (3-n_i(G))n_j(G)(\Phi(\{n_k(G')\}_{k\in\Lambda}), \Phi(\{n_k(G)+\delta_{k,i}-\delta_{k,j}\}_{k\in\Lambda}))\\ &= \sum_{G',G} \prod_{k\in\Lambda} \chi(n_k(G')=n_k(G)+\delta_{k,i}-\delta_{k,j})(n_k(G)+\delta_{k,i})!\,(3-n_k(G)+\delta_{k,j})!\,.\end{aligned} \tag{3.13}$$

Again we represent the above formula geometrically. This time, the same number of straight and wavy segments must be incident to each site in Λ except i and j. At site i we must have one extra wavy segment, and at site j we must have one extra straight segment (Fig. 3.3b). This observation allows us to construct a self-avoiding random walk connecting i and j as follows.

Consider an arbitrary pair of G', G which contributes to (3.13), and the corresponding graph of straight and wavy segments. Then from the above property we can find at least one bond (i, k_1) which is occupied *only* by a wavy segment (Fig. 3.3b). [If there exist more than one (i.e., two) such bonds, we choose one of them by a suitable convention.] If $k_1 \neq j$, there are equal numbers of straight and wavy segments incident to k_1. Since the bond (k_1, i) is occupied only by a wavy segment, this implies that there exists a *unique* bond (k_1, k_2) occupied only by a straight segment. By repeating the same procedure, we get a sequence of bonds (i, k_1), (k_1, k_2), (k_2, k_3), ... occupied only by straight or wavy segments in an alternating way (Fig. 3.3b). Clearly, this sequence terminates only when we hit the site j, and thus it forms a self-avoiding walk $\omega = \{k_0, k_1, \ldots, k_n\}$, where $k_0 = i$, $k_n = j$, $(k_i, k_{i+1}) \in \mathbb{B}$ for any i, and $k_l \neq k_m$ if $l \neq m$. We stress that such a self-avoiding walk is always determined *uniquely* from any pair G', G which contributes to (3.13), if we fix a convention for the choice of the first step of the walk at site i. Let us denote this unique self-avoiding walk by $\omega(G', G)$.

Now from (3.11), (3.13), and the above construction, we can write down the following *random walk representation* for the two point correlation function:

$$\langle S^+{}_i S^-{}_j \rangle = \frac{(\Omega_\Lambda, S^+{}_i S^-{}_j \Omega_\Lambda)}{(\Omega_\Lambda, \Omega_\Lambda)} = \sum_{\omega: i\to j} W(\omega). \tag{3.14}$$

Here ω runs over all the self-avoiding walks on the lattice connecting i and j, and the statistical weight $W(\omega)$ is defined by

$$W(\omega) = \frac{\sum_{G',G\subset\mathbb{B}} \chi(\omega(G',G)=\omega) \prod_{k\in\Lambda} \chi(n_k(G')=n_k(G)+\delta_{k,i}-\delta_{k,j})(n_k(G)+\delta_{k,i})!(3-n_k(G)+\delta_{k,j})!}{\sum_{G',G\subset\mathbb{B}} \prod_{k\in\Lambda} \chi(n_k(G')=n_k(G))n_k(G)!\,(3-n_k(G))!}. \tag{3.15}$$

When i and j are not both in Λ_B, we can also carry out the same construction and get similar random walk representations. Here the weight $W(\omega)$ has an overall factor $(-1)^{i-j}$ which comes from the analog of (3.12) for sites in Λ_A.

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In the following we will show that for any ω this statistical weight can be bounded as

$$W(\omega) \leqq C_1(\sqrt{6})^{-|\omega|}, \tag{3.16}$$

where $|\omega|$ denotes the length of the walk ω (i.e., the number of bonds in ω), and C_1 is a finite constant independent of the lattice size.

Combining (3.14) and (3.16) we get

$$\langle S^+{}_i S^-{}_j \rangle \leqq C_1 \sum_{\omega: i \to j} (\sqrt{6})^{-|\omega|} \leqq C_1 \sum_{l=|i-j|}^{\infty} N(l)(\sqrt{6})^{-l},$$

where $N(l)$ denotes the number of distinct self-avoiding walks with length l. Since the coordination number of the lattice is three, $N(l)$ can be bounded by its mean field behavior as $N(l) \leqq 2^l$. Inserting this bound in the above inequality and summing over l, we get

$$\langle S^+{}_i S^-{}_j \rangle \leqq C_2 \exp(-|i-j|/\xi_0),$$

where $\xi_0 = \{\ln(2/\sqrt{6})\}^{-1} = 4.93\ldots$, and $0 < C_2 < \infty$ is independent of the lattice size. Since $\langle S^+{}_i S^-{}_j \rangle = (\langle S^1{}_i S^1{}_j \rangle + \langle S^2{}_i S^2{}_j \rangle)/4$, the $SO(3)$ symmetry of the system implies the desired bound (3.6) for the correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$. For the hexagonal lattice, the exact (but nonrigorous) behavior of $N(l)$ is known to be $N(l) = (\sqrt{2+\sqrt{2}})^{l+o(l)}$ [33]. Using this instead of the above crude mean field upper bound, we get an improved upper bound $\xi_1 = 3.54\ldots$ for the correlation length.

Now let us turn to the proof of the bound (3.16) for the statistical weight of the random walks. Fix a random walk ω. Denote the numerator and denominator of (3.15) by Z_ω and Z, respectively. We will construct a lower bound for Z in terms of Z_ω. Consider a graph for a pair G', G which contributes to Z_ω. If we eliminate all the segments in the graph which are on the walk ω, we will get a graph in which the same numbers of straight and wavy segments are incident to any site. Moreover, this property is preserved if we put both a straight and a wavy segment on any bond in the trajectory of the eliminated walk ω. In this way, we get $2^{|\omega|}$ distinct graphs which contribute to the norm Z (Fig. 3.4a–c). Note that given any one of these $2^{|\omega|}$ graphs we can recover G', G. (Recall that ω is fixed.) Thus each term in Z appears at most once as one of these $2^{|\omega|}$ graphs for some G', G.

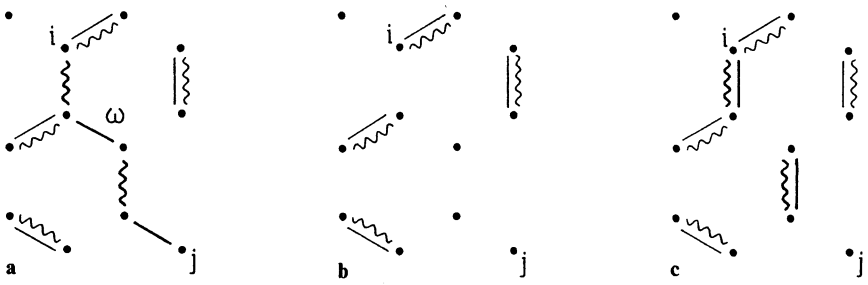

Fig. 3.4. **a** A typical term in Z_ω. **b** The result of deleting the lines in ω. **c** One of the $2^{|\omega|}$ terms in Z which are associated with **a**

We have shown that with each term G', G in Z_ω we may associate $2^{|\omega|}$ terms in Z. These $2^{|\omega|}$ terms need not have the same weight as the original term in Z_ω. To compare the weights, first note that the local weights $n_k(G)!\,(3-n_k(G))!$ and $(n_k(G)+\delta_{k,i})!\,(3-n_k(G)+\delta_{k,j})!$ only take on the values 3! and 2! for sites $k \neq i, j$. For a site $k \neq i, j$ which belongs to ω, $n_k(G)$ must be 1 or 2, so the local weight $n_k(G)!\,(3-n_k(G))!$ equals 2!. Thus the weight appearing in Z_ω is always less than or equal to the weight appearing in Z. This yields the bound

$$Z \geqq \text{const}\, 2^{|\omega|} Z_\omega .$$

To obtain the stronger bound (3.16) we need to take advantage of the fact that the local weight in Z is sometimes 3!. At the sites $k_2, k_4, k_6, \ldots$ we simply bound the local weight in Z below by 2!. Let k be one of the sites $k_3, k_5, \ldots$ other than j. The bond incident to k which does not belong to ω must either be empty or contain both a straight and a wavy segment. Suppose it is empty. Then when both of the bonds in ω incident to k are empty, the local weight at k for the term in Z is 3!. If at least one of the bonds in ω incident to k has both a straight and wavy segment, then the local weight is 2!. Thus out of the four possibilities for the two bonds in ω incident to k, exactly three have a local weight of 2! and exactly one has a local weight of 3!. If the bond incident to k which is not on ω contains both a straight and a wavy segment, then we find the same conclusion is true. Hence for every two bonds in ω, we obtain a factor of $3+3\cdot 1=6$, instead of just $2\cdot 2=4$. Inequality (3.16) follows.

4. VBS States on an Arbitrary Lattice

4.1. The Ground States

In the present section, we extend the VBS state to an arbitrary lattice, and discuss its properties.

Let Λ be the set of sites in a translation invariant finite lattice with periodic boundary conditions and coordination number z. The set of bonds $\mathbb{B}$ consists of unordered pairs (i, j) of adjacent sites i, j in Λ. We also assume that the lattice is bipartite, i.e., it can be decomposed into two sublattices Λ_A, Λ_B with the properties $\Lambda_A \cup \Lambda_B = \Lambda$, $\Lambda_A \cap \Lambda_B = \emptyset$ and for any $(i, j) \in \mathbb{B}$, either $i \in \Lambda_A$, $j \in \Lambda_B$ or $j \in \Lambda_A$, $i \in \Lambda_B$.

Let us associate a spin operator $\mathbf{S}_i$ with spin $s = z/2$ with site i. Consider the $SO(3)$ symmetric antiferromagnetic Hamiltonian

$$H = \sum_{(i,j)\in\mathbb{B}} P_z(\mathbf{S}_i + \mathbf{S}_j) = \sum_{(i,j)\in\mathbb{B}} H_{ij}, \tag{4.1}$$

where $P_z(\mathbf{S})$ is the orthogonal projection onto the states with $\mathbf{S}^2 = z(z+1)$ (spin z).

The VBS ground state is again constructed by first regarding spin $z/2$ as the symmetric part of the product of z spin 1/2's, and then letting each pair of spin 1/2's on the adjacent sites form a singlet pair. In this way, the valence bond structure again becomes identical to the bond structure $\mathbb{B}$ of the lattice.

To describe the VBS state precisely, we again make use of an $SU(2)$ notation. For a single spin with $s = z/2$, our basis consists of the following vectors with $\alpha_i = 1$ or 2:

$$\psi_{\alpha_1 \ldots \alpha_z} = \sum_{(\alpha_1, \ldots, \alpha_z) \to (\beta_1, \ldots, \beta_z)} \psi_{\beta_1} \otimes \ldots \otimes \psi_{\beta_z} / \sqrt{z!}\,. \tag{4.2}$$

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Here $\{\psi_1=(+), \psi_2(-)\}$ denotes the standard S^3 eigenstate basis for an $s=1/2$ spin, and the summation runs over all the permutations of $(\alpha_1, \ldots, \alpha_z)$. These states satisfy the following normalization condition:

$$(\psi_{\alpha_1 \ldots \alpha_z}, \psi_{\beta_1 \ldots \beta_z}) = \sum_{(\beta_1, \ldots, \beta_z) \to (\gamma_1, \ldots, \gamma_z)} \delta_{\alpha_1 \gamma_1} \delta_{\alpha_2 \gamma_2} \ldots \delta_{\alpha_z \gamma_z}. \tag{4.3}$$

Let $i_1, \ldots, i_z$ denote the z neighboring sites of a site i. We represent a state on site i as

$$\psi_{\alpha_{ii_1} \alpha_{ii_2} \ldots \alpha_{ii_z}}$$

if $i \in \Lambda_A$, and as

$$\psi^{\alpha_{ii_1} \alpha_{ii_2} \ldots \alpha_{ii_z}}$$

if $i \in \Lambda_B$. Here the state with the raised indices is defined as before. Then the VBS state on the general lattice Λ can be expressed as

$$\Omega_\Lambda = \bigotimes_{i \in \Lambda_A} \psi_{\alpha_{ii_1} \alpha_{ii_2} \ldots \alpha_{ii_z}} \bigotimes_{j \in \Lambda_B} \psi^{\alpha_{jj_1} \alpha_{jj_2} \ldots \alpha_{jj_z}}. \tag{4.4}$$

As in Sect. 3.1, we identify α_{ij} with α_{ji}, and sum over all the repeated upper and lower indices. Then all the indices in (4.4) are contracted, and we get a single state Ω_Λ. Again it is quite easy to check that the VBS state (4.4) is an exact ground state of the Hamiltonian (4.1) in the sense that $H_{ij}\Omega_\Lambda = 0$ holds for any $(i, j) \in \mathbb{B}$.

As in the hexagonal lattice VBS state, we do not have any uniqueness argument like Theorem 2.7. Though we believe that an analog of Lemma 2.8 (finite volume lemma) is true, the uniqueness in the infinite volume limit seems not to be true in general. We return to this point later.

In Sects. 2 and 3, we have seen that the VBS state on the one-dimensional chain and two-dimensional hexagonal lattice seem to share common properties, namely, the exponential decay of correlations, the absence of Néel order, and the existence of an energy gap. Thus one might well conclude that these are general features of all VBS states. However, in the following subsections we will present a Cayley tree model and a stochastic geometric argument which suggest this is not the case. As we summarize in the following conjecture, the VBS state on certain lattices may be in a completely different phase.

Conjecture. If the coordination number z and the dimension d are sufficiently small, the system (4.1) is in the *VBS phase*, i.e., it has a unique (infinite volume) ground state with exponentially decaying correlation functions, no Néel order, and a finite energy gap. However, if z and d are sufficiently large, the system (4.1) is in the Néel ordered phase.

As we have noted in the previous section, we expect (but cannot prove) that the VBS state does not have Néel order if the coordination number of the lattice is three. Since we can construct a lattice with coordination number three in any dimension d, not only large d but also large z is actually necessary for the existence of Néel order.

When the system is in the Néel ordered phase, the infinite volume limit of the VBS state (4.4) constructed using periodic boundary conditions cannot be a pure

state since this VBS state has no $SO(3)$ symmetry breaking. A pure state with explicit Néel order may be obtained by the following procedure. Consider a finite lattice Λ with boundary $\partial\Lambda$, and construct the VBS state on Λ. The only difference from the periodic boundary condition case (4.4) is that at each site in $\partial\Lambda$ several spin 1/2's remain uncontracted. It is clear that for any choice of these boundary spin 1/2's, the VBS state is an exact ground state in the sense that $H_{ij}\Omega_\Lambda = 0$ for any bond (i, j). Consider the boundary conditions where we fix the boundary spin 1/2's to $(+)$ for the sites in $\partial\Lambda \cap \Lambda_A$, and to $(-)$ for the sites in $\partial\Lambda \cap \Lambda_B$. By taking the infinite volume limit of the VBS states with these boundary conditions, we should get a pure ground state with nonzero staggered magnetization, provided that the system is in the Néel ordered phase. In the next subsection, we will carry out this procedure for the Cayley tree and show that there is Néel order when the coordination number exceeds four.

The existence of Néel order in valence bond states is not as surprising as it appears. Though a valence bond carries strong quantum fluctuations, it also has a tendency to make the two spins "point" in opposite directions. The behavior of the VBS (or other valence bond) states in the infinite volume limit is determined by the competition of these two effects.

4.2. The VBS State on the Cayley Tree

In the present subsection, we describe our results on the VBS state on the Cayley tree. Let C_N be the N-th order Cayley tree with coordination number z (Fig. 4.1a), and ∂C_N be its boundary. We assume N is even. Again we decompose C_N into two sublattices Λ_A and Λ_B, so that the boundary ∂C_N and the origin are contained in the sublattice Λ_B. Then the VBS state on the Cayley tree is

$$\Omega_N = \bigotimes_{i\in\Lambda_A} \psi_{\alpha_{ii_1}\alpha_{ii_2}\cdots\alpha_{ii_z}} \bigotimes_{j\in\Lambda_B\setminus\partial C_N} \psi^{\alpha_{jj_1}\alpha_{jj_2}\cdots\alpha_{jj_z}} \bigotimes_{k\in\partial C_N} \psi^{\alpha_{kk_1}22\cdots2}. \tag{4.5}$$

In order to test for the existence of Néel order, we have set the boundary $s=1/2$ spins to $(+)$.

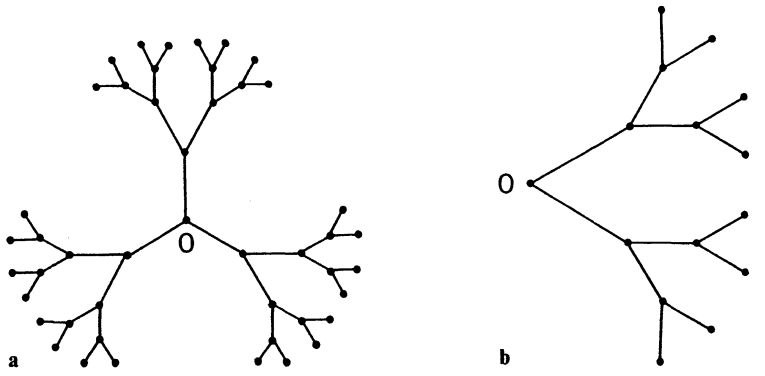

Fig. 4.1. **a** The fourth order Cayley tree C_4 with coordination number three, and **b** the corresponding branch B_4

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Let us define the *Néel order parameter* by

$$m = \lim_{N\to\infty} \frac{(\Omega_N, S_0{}^3\Omega_N)}{(\Omega_N, \Omega_N)}, \tag{4.6}$$

where $S_0{}^3$ is the third (z-) component of the spin operator at the origin (center of the Cayley tree). As we describe later, we find that the Néel order parameter m is vanishing for $z=3$, and is strictly positive for $z>4$. For $z=4$ numerical calculations indicate the order parameter vanishes, but we have not produced a rigorous proof from these calculations. Note that this is consistent with our conjecture in the previous subsection.

It is also not difficult to show that in the infinite Cayley tree with any z and *free boundary conditions*, the two point function always decays exponentially as

$$\langle \mathbf{S}_0 \cdot \mathbf{S}_x \rangle \sim (-3)^{-|x|}, \tag{4.7}$$

where $|x|$ is the graph theoretic distance (the number of the bonds between 0 and x). It may seem that this is inconsistent with the above mentioned Néel order for $z>4$. However, this exponential decay for free boundary conditions is nothing but a pathological feature commonly found in Cayley tree systems. It is due to the exponential increase of the number of neighbors within a fixed distance, and has nothing to do with the existence or absence of Néel order. Moreover, the following quantity indicates the marginality of $z=4$.

$$\sum (-1)^{|x|} \langle \mathbf{S}_0 \cdot \mathbf{S}_x \rangle \begin{cases} <\infty & \text{for } z<4, \\ =\infty & \text{for } z \geqq 4. \end{cases}$$

Finally, we consider the mixed boundary conditions as in Fig. 4.2 which favor the existence of a *domain wall* between two regions which have opposite Néel orders. The VBS state with these boundary conditions also satisfies the condition $H_{ij}\Omega_A = 0$ for any bond (i, j). Unlike the standard models (e.g., Ising or usual Heisenberg models) the domain wall (in the finite system) in the VBS state does not cost any energy.

Let us denote the infinite volume limit of the above state (Fig. 4.2) by $\varrho_\pm$. We can show that, for an even $z>4$, $\varrho_\pm$ contains a domain wall in the sense that $(-1)^i \varrho_\pm(S_i{}^3) < 0$ when i is in a branch with the plus boundaries, and $(-1)^i \varrho_\pm(S_i{}^3) > 0$ when i is in a branch with the minus boundaries. Since the state satisfies $\varrho_\pm(H_{ij}) = 0$ for any bond (i, j), the domain wall costs no energy. This raises the possibility that the VBS state with such a zero energy domain wall exists in the regular lattice when the system is in the Néel ordered phase and the dimension is sufficiently high.

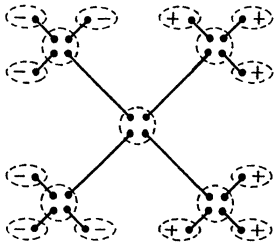

Fig. 4.2. Boundary conditions which favor the existence of a domain wall. + (or −) stands for the three spin 1/2's at the boundary

Derivation of the Results. We now show that the Néel order parameter vanishes for $z=3$ and is strictly positive for $z>4$.

Note that the formula (3.11) for the norm of the VBS state can be easily extended to the general VBS state as follows:

$$(\Omega_\Lambda, \Omega_\Lambda)=\sum_{G', G\subset \mathbf{B}} \prod_{k\in\Lambda} \chi(n_k(G')=n_k(G)) n_k(G)!\,(z-n_k(G))!\,.$$

Since the Cayley tree contains no loops, the only way to satisfy $n_k(G')=n_k(G)$ for all k is to set $G'=G$. Thus the above formula simplifies to

$$(\Omega_N, \Omega_N)=\sum_{G\subset \mathbf{B}} \prod_{k\in C_N} n_k(G)!\,(z-n_k(G))!\,, \tag{4.8}$$

where G runs over all subsets of the bonds in C_N, and $n_k(G)$ is the number of bonds in G which are incident to k.

Let B_M be a branch in the Cayley tree C_M where M is an arbitrary integer (Fig. 4.1b). To evaluate the sum (4.8), let us define the following quantities:

$$Y_M=\sum_G (n_0(G)+1)!\,(z-n_0(G)-1)! \prod_{k\in B_M\setminus 0} n_k(G)!\,(z-n_k(G))!\,,$$

$$Z_M=\sum_G \prod_{k\in B_M} n_k(G)!\,(z-n_k(G))!\,,$$

where 0 denotes the origin of the branch B_M (see Fig. 4.1b). Note that Y_M and Z_M represent the norms of the VBS states on B_M which have plus boundary condition and minus boundary condition, respectively, at the origin. Both states have minus (respectively plus) boundary conditions at all the other boundary sites when M is even (respectively odd). Their "initial values" are given by $Y_1=(z-1)!$ and $Z_1=z!$.

The lattice B_{M+1} can be constructed by gluing together one bond and $(z-1)$ copies of B_M at a vertex order z. Noting that we can assign either Y_M or Z_M to each B_M, we get the following recursion equation:

$$\begin{aligned} Y_{M+1}&=\sum_{i=0}^{z-1}\binom{z-1}{i}(Y_M)^i(Z_M)^{z-1-i}(i+1)!\,(z-1-i)! \\ &=(z-1)!\sum_{i=0}^{z-1}(i+1)(Y_M)^i(Z_M)^{z-1-i}. \end{aligned}$$

The recursion equation for Z can be obtained in a similar way,

$$Z_{M+1}=(z-1)!\sum_{i=0}^{z-1}(z-i)(Y_M)^i(Z_M)^{z-1-i}.$$

Let us define a new quantity W_M by $W_M=Y_M/Z_M$. From the recursion equations for Y_M and Z_M, we get

$$W_{M+1}=f_z(W_M), \tag{4.9}$$

where

$$f_z(W)=\frac{\sum_{i=0}^{z-1}(i+1)W^i}{\sum_{i=0}^{z-1}(z-i)W^i}. \tag{4.9'}$$

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Therefore, we can find the value of W_M by starting from the initial value $W_1 = 1/z$, and applying the above one-dimensional map $f_z(\cdot)$ $M-1$ times. In the infinite volume limit the calculation reduces to the following elementary fixed point analysis.

Note that the map $f_z(W)$ satisfies the following properties:

i) $f_z(W)$ is continuous for $W>0$.

ii) $f_z(W)$ is monotone nondecreasing for $W>0$. (To see this, note that $f_z'(W) = C \sum_{i,j=1,\ldots,z-1} (i^2-ij)W^{i+j} = C \sum_{i,j=1,\ldots,z-1} \{(i-j)^2/2\} W^{i+j} \geqq 0$, where C is a positive quantity.)

iii) $1/z \leqq f_z(W) \leqq z$ for $W>0$. (This follows from i) and $f_z(0)=1/z$, $\lim_{W\to\infty} f_z(W) = z$.)

From i)–iii), it follows that the limit

$$W_\infty = \lim_{M\to\infty} W_M = \lim_{M\to\infty} f_z^M(1/z)$$

always exists and is determined by the fixed point to which the initial value $W=1/z$ is attracted. [*Proof.* Let $W_1 = 1/z$. By iii), $W_2 \geqq W_1$. Because of ii) we then have $W_3 \geqq W_2 \Rightarrow W_4 \geqq W_3 \Rightarrow$ etc. Therefore, $\{W_M\}$ is a bounded increasing sequence and hence has a limit.]

Clearly, the map $f_z(W)$ has $W=1$ as a fixed point. Since the gradient of $f_z(W)$ at $W=1$ is $f_z'(1) = (z-1)/3$, this fixed point is *stable* if $z<4$, and *unstable* if $z>4$. Thus for $z>4$, the initial value $W=1/z$ cannot be deriven to the fixed point $W=1$. Moreover, from the properties i)–iii), we can conclude the following:

$$0 < W_\infty < 1 \quad \text{for} \quad z>4. \tag{4.10}$$

For $z=3$, we can show the following property of $f_z(W)$ (by a brute force calculation).

iv) $f_3''(W) \geqq 0$ holds for $1/3 \leqq W \leqq 1$.

Therefore, the initial value $W=1/3$ must be attracted to the fixed point $W=1$. Thus we have

$$W_\infty = 1 \quad \text{for} \quad z=3. \tag{4.11}$$

For $z=4$, the fixed point $W=1$ is marginally stable. We expect (based on numerical calculations) that the initial value $W=1/4$ is driven to this fixed point, and $W_\infty = 1$ holds.

It is not difficult to find that the expectation value for $S_0{}^3$ can be expressed in terms of W_∞ as

$$m_z = \lim_{N\to\infty} \langle S_0{}^3 \rangle_{z,N} = \frac{\sum_{i=0}^{z} (z/2-i)(W_\infty)^i}{\sum_{i=0}^{z} (W_\infty)^i}.$$

Substituting the values of W_∞ (4.10), (4.11) into the above formula, we get the desired result:

$$m=0 \quad \text{if} \quad z=3,$$
$$m>0 \quad \text{if} \quad z>4.$$

Numerical calculations yield the following values of the (normalized) Néel order parameters:

$$m/s=0, \qquad z=4,$$
$$=0.814\ldots, \qquad z=5,$$
$$=0.902\ldots, \qquad z=6.$$

To get the estimate (4.7) for the correlation function, note that, for free boundary conditions, we have $W_1=1$ and thus $W_M=1$ for any M and z. Therefore, the formula for correlation functions becomes quite simple. Then the desired (4.7) can be derived from a representation similar to (3.14) and a little calculation.

Finally, the result on the zero energy domain wall is a simple consequence of the fact that $W_\infty<1$ for the plus boundary conditions, and $W_\infty>1$ for the minus boundary conditions if $z>4$.

4.3. SU(N) VBS State and Random Loop Representation

Here we will describe a set of heuristic and rigorous results which provide further support for our conjecture (that there is Néel order in the VBS state if the coordination number and dimension are both large and there is none if they are both small) in Sect. 4.1. Two keys for the arguments developed here are $SU(N)$ generalizations of the VBS states, and a random loop representation for the correlation functions. This random loop representation should not be confused with the random walk representation in Sect. 3.3. It is interesting that the VBS state has two natural geometric representations.

First, let us formally extend the VBS state (4.4) to the $SU(n)$ quantum "spin" system [2]. More detailed discussion about the $SU(n)$ generalizations will be given in the next subsection. To get the $SU(n)$ VBS state, we simply let the indices α_{ij} in (4.4) run from 1 to n, instead of 1 to 2. The basis vectors $\psi_{\alpha_1\alpha_2\ldots\alpha_z}$ still satisfy the normalization condition (4.3) where $\delta_{\alpha\beta}$ should be regarded as the n by n unit matrix.

In the one-dimensional model, the calculation of the correlation function presented in Sect. 2.2 generalizes easily to arbitrary n. The basic formula for the action of the spin operators (2.15) is still valid for the $SU(n)$ model, if we regard $\sigma_\alpha{}^\beta$ as the $SU(n)$ generalization of the Pauli matrices, i.e., a basis of the Lie algebra chosen so that $\mathrm{Tr}\,\sigma^a\sigma^b=(\sigma^a)_\alpha{}^\beta(\sigma^b)_\beta{}^\alpha=2\delta^{ab}$. Then everything is the same as before but now there is a factor of n for each loop instead of 2 as for $SU(2)$. Thus the normalization of the open chain of length L becomes

$$\Omega^{\dagger\alpha}{}_\beta\cdot\Omega_\gamma{}^\delta=\delta^\alpha{}_\gamma\delta^\delta{}_\beta\{(n+1)^L-1\}/n+\delta^\alpha{}_\beta\delta^\delta{}_\gamma.$$

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For the closed chain we obtain $(n+1)^L-1+n^2$. The correlation function is

$$\langle S^a{}_0 S^b{}_r\rangle = (-1)^r(1/2)^2 2\delta^{ab}[2(n+1)^{L-r}+(n+1)^{L-r-1}+(n+1)^{L-r+1}]/n(n+1)^L$$
$$= (-1)^r[(n+2)^2/2n(n+1)](n+1)^{-r} \quad (\text{for } r>1)$$

for $a,b=1,\ldots,n^2-1$. Note that the correlation length, $1/\ln(n+1)$, is finite for all $n>0$, and diverges as $n\to 0$. Thus the $SU(n)$ VBS state in the one-dimensional lattice is in the VBS phase for all $n>0$.

In the Cayley tree model, we can again construct recursion equations for the n quantities corresponding to Y_M, Z_M, and carry out a fixed point analysis similar to (but a little more complicated than) the $SU(2)$ case. Then we find that the trivial fixed point representing the VBS phase [like $W=1$ in the $SU(2)$ case] is stable in the region $(z-1)/(n+1)<1$. Therefore, the $SU(n)$ VBS state is in the VBS phase for $z\geqq n+2$, and in the Néel ordered phase for $z<n+2$. This is consistent with the one-dimensional case where $z=2$ and the critical value of n is zero.

In order to get some idea of the phase diagram for the $SU(n)$ VBS state on regular lattices, we construct a stochastic geometric representation for the correlation functions. The representation is essentially a straightforward extension of the diagramatic method used in Sect. 2.2.

Let Λ be an arbitrary finite bipartite lattice with coordination number z. To compute the norm of the $SU(n)$ VBS state Ω_Λ we apply (4.3) to each site in the representation (4.4) of Ω_Λ. The result is that $(\Omega_\Lambda,\Omega_\Lambda)=\Omega_\Lambda{}^\dagger\cdot\Omega_\Lambda$ is a sum of $(z!)^{|\Lambda|}$ terms. To obtain a diagramatic representation of this sum we first represent Ω_Λ as shown in Fig. 4.3, where we have assigned a direction to each bond in such a way that the bond points from a site in Λ_A to a site in Λ_B. We represent $\Omega_\Lambda{}^\dagger$ by the same graph with the direction of every bond reversed. We now place the graphs for Ω_Λ and $\Omega_\Lambda{}^\dagger$ on top of each other. One term in the sum (4.3) is represented by pairing each bond coming into the vertex with a bond going out of the vertex. Two bonds that hit a vertex are considered to be attached only if they are paired together. For example, with $z=3$ the 3! terms for a single vertex are represented by Fig. 4.4. In this way each term in $(\Omega_\Lambda,\Omega_\Lambda)=\Omega_\Lambda{}^\dagger\cdot\Omega_\Lambda$ is represented by a collection of loops on the lattice. The contribution from a single loop is $\delta_{\alpha_1}{}^{\alpha_2}\delta_{\alpha_2}{}^{\alpha_3}\ldots\delta_{\alpha_m}{}^{\alpha_1}=n$. Thus

$$\Omega_\Lambda{}^\dagger\cdot\Omega_\Lambda=\sum_C n^{\#C}, \tag{4.12}$$

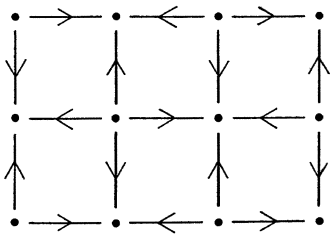

Fig. 4.3.

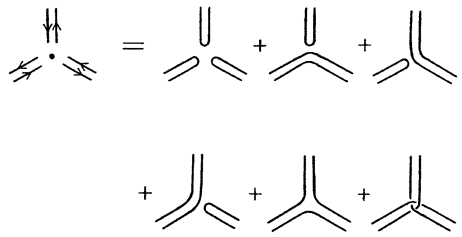

Fig. 4.4.

Fig. 4.3. Diagramatic representation of Ω_Λ

Fig. 4.4. Diagramatic rule used in calculating the overlaps

where $\#C$ is the number of distinct loops in the configuration C, and the sum is over all configurations of loops on the lattice with the property that each bond in the lattice is covered exactly twice by C.

To get the expression for the correlation functions, we generalize (2.15) to general spin s as

$$S\psi_{\alpha_1\alpha_2\ldots\alpha_z} = -\frac{1}{2}\sum_{k=1}^{z} \sigma_{\alpha_k}{}^{\beta}\psi_{\alpha_1\alpha_2\ldots\hat{\alpha}_k\ldots\alpha_z\beta},$$

where $\hat{\alpha}_k$ is an omitted index, and $\sigma_\alpha{}^\beta$ again denotes the $SU(n)$ version of the Pauli matrices. Combining this formula with (4.4), we can again express the unnormalized correlation functions in terms of the random loop configurations as

$$\Omega_\Lambda{}^\dagger \cdot \mathbf{S}_i \cdot \mathbf{S}_j \Omega_\Lambda = (-1)^{i-j}/4 \sum_{\substack{b \ni i \\ b' \ni j}} \sum_{C} \chi(b \text{ and } b' \text{ belong to the same loop}) n^{\#C}. \tag{4.13}$$

Here the characteristic function $\chi(A)$ equals 1 if A is true, and 0 if A is false. b (respectively b') runs over the bonds in the graph of Ω_Λ which contain i (respectively j). The prefactor $(-1)^{i-j}$ is 1 if i and j belong to the same sublattice, and -1 otherwise. We have assumed that i and j are separated by a distance >1.

From (4.12) and (4.13) we get the following *random loop representation* for the correlation function.

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\Lambda,n} = (-1)^{i-j}/4 \sum_{\substack{b \ni i \\ b' \ni j}} \mathrm{Prob}_{\Lambda,n}(b \text{ and } b' \text{ belong to the same loop}). \tag{4.14}$$

Here the probability for the basic event that a particular random loop configuration C is present is defined to be

$$\mathrm{Prob}_{\Lambda,n}(C) = n^{\#C} \Big/ \sum_{C'} n^{\#C'}. \tag{4.15}$$

Note that, in the above definition, the logarithm of n can be regarded as the *chemical potential* for the loops in our stochastic geometric system. By (4.14) and (4.15), we are now able to extend the correlation function for $SU(n)$ VBS state to noninteger (complex!) values of n. In the following analysis, we regard (4.14) and (4.15) as our starting points, and consider positive but not necessarily integer n.

For large values of n, the configurations with many loops (as in Fig. 4.5a) are favored by (4.15). We expect that the random loop system is in the *nonpercolating phase* where the loops are localized and have finite size (with probability one). In particular, the probability that two sufficiently separated bonds belong to the same loop is expected to decay exponentially with the distance between the bonds. Thus the $SU(n)$ VBS state should be in the VBS phase which has short range correlations.

For small values of n, the configurations with large loops (as in Fig. 4.5b) are the main contribution to (4.13), (4.14). Then the random loop system (in the infinite volume limit) may be in the *percolating phase* where a (unique) infinite loop appears in the configuration (with probability one). If the probability that a bond belongs to the infinite loop is strictly positive, (4.14) suggests that the two point correlation function $|\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|$ is bounded below by this probability squared.

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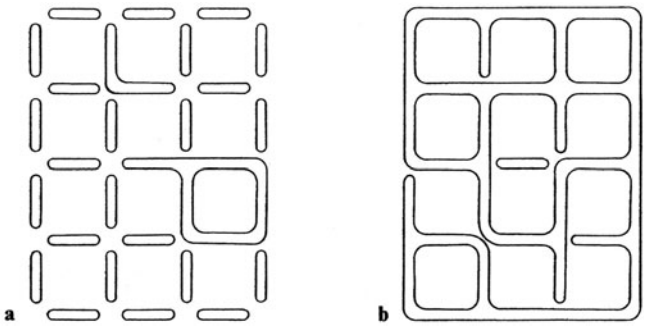


Fig. 4.5. Typical diagrams which contribute to $\Omega_A^{\dagger} \cdot \Omega_A$ for **a** large n (nonpercolating phase) and **b** small n (percolating phase)

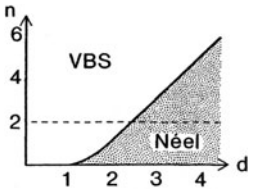


Fig. 4.6. Conjectured phase diagram for the $SU(n)$ VBS states

Therefore, the $SU(n)$ VBS state is expected to be in the Néel ordered phase. Of course, this is not true for the one-dimensional chain, where the VBS phase exist for all $n>0$. However, this simply reflects the special character of the marginal one-dimensional lattice, where there are relatively few infinite loops.

In the general infinite lattice, therefore, we conjecture that there exists a critical value n_c ($\geqq 0$). The $SU(n)$ VBS state is in the VBS phase (which corresponds to the nonpercolating phase) for $n>n_c$, and is in the Néel ordered phase (which corresponds to the percolating phase) for $n<n_c$. The critical value n_c is exactly known only for the Cayley tree model where $n_c=z-2$ and for the one-dimensional lattice where $n_c=0$. We expect that this Cayley tree value becomes reliable in higher dimensions. In Fig. 4.6, we summarize our conjectured phase diagram for the $SU(n)$ VBS state on the d-dimensional hypercubic lattice. This phase diagram, when restricted to $n=2$, again suggests the existence of a transition from the VBS phase to the Néel ordered phase as the dimension is increased. Thus it provides further support for our conjecture in Sect. 4.1.

It is desirable to have rigorous arguments which support the above heuristic discussion about the $SU(n)$ VBS state. At present we can only prove the following proposition which confirms our picture for sufficiently large values of n. The proof of the existence of Néel order for sufficiently small n is probably difficult since it involves continuous symmetry breaking. We also note that Theorem 3.1 proves the upper bound $n_c<2$ for any bipartite lattice with coordination number three.

Proposition 4.1. *Consider an arbitrary (infinite) bipartite lattice with coordination number z. If* $n>(z!)^{2(z-1)}$, *the SU(n) VBS state on the lattice is in the VBS phase, i.e.,*

every truncated correlation function decays exponentially, and there is no Néel order.

Proof. Consider a finite lattice, and let l be a loop which contains a fixed bond b_0 in the graph of Ω_Λ. The statistical weight for a single loop l is defined as

$$\omega(l)=\sum_{C\ni l} n^{\#C}\Big/\sum_{C} n^{\#C}.$$

In the following we prove that $\omega(l)$ can be bounded uniformly in the lattice size as

$$\omega(l)\leqq n\{(z-1)!\,(z!)^{z-2}/\sqrt{n}\}^{|l|},$$

where $|l|$ is the length (number of bonds) of l. From this bound and the representation (4.14), we get the following upper bound for the two point correlation function provided that $n>(z!)^{2(z-1)}$:

$$\begin{aligned}\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle &\leqq z^2\,\mathrm{Prob}(|l|\geqq 2(|i-j|-2))\\ &\leqq \sum_{k=2(|i-j|-2)}^{\infty} z^k n\{(z-1)!\,(z!)^{z-2}/\sqrt{n}\}^k = C\exp(-|i-j|/\xi_0).\end{aligned}$$

Here $0<C,\ \xi_0<\infty$ are independent of the lattice size. We have bounded the number of the loops with $|l|=k$ by z^k in the above.

To prove the asserted bound for $\omega(l)$, consider an arbitrary loop l and denote by $\hat{l}$ the set of all the lattice bonds which belong to or are incident to l. Given a loop configuration $C\ni l$, we replace the loop configuration on $\hat{l}$ by a collection of minimum single bond loops to construct a new configuration $\hat{C}$. Clearly, $\hat{C}$ contains at least $|l|/2-1$ more loops than C does. Noting that at most $(z-1)!^{|l|}(z!)^{(z-2)|l|}$ different C can be mapped into a single $\hat{C}$ (because of the redundant freedom in $\hat{l}$), we get

$$n^{|l|/2-1}\sum_{C\ni l} n^{\#C}/(z-1)!^{|l|}(z!)^{(z-2)|l|}\leqq \sum_{C} n^{\#C},$$

which implies the desired bound for $\omega(l)$. The exponential decay of every truncated correlation function and the absence of Néel order can be proved by the same estimates. □

4.4. SU(n) Quantum "Spin" System

In the present subsection we amplify the discussions of the $SU(n)$ VBS state in the previous subsection by presenting some details of the $SU(n)$ quantum "spin" systems which were first introduced in [2].

Consider the simplest $s=1/2$ case. As we have noted several times, we denote the standard S^3 eigenstates $(+)$ and $(-)$ by ψ_α, $\alpha=1,2$, respectively. To generalize this basis from $SU(2)$ to $SU(n)$, we simply let the index α run from 1 to n. Then the basis for a finite bipartite lattice again consists of the simple tensor product of ψ_α on one sublattice and ψ^α on the other sublattice. This corresponds to putting the fundamental representation of $SU(n)$ on one sublattice, and its conjugate representation on the other. Again the $SU(n)$ singlet (valence bond) can be simply represented as $\psi_\alpha{}^\alpha$ $(=\psi_\alpha\otimes\psi^\alpha)$.

Valence Bond Ground States in Isotropic Quantum Antiferromagnets

To get the $SU(n)$ generalization of the Hamiltonian, it is useful to represent the action of the Hamiltonian in terms of the valence bond basis. Note that in the $SU(2)$ case, the $s=1/2$ Heisenberg Hamiltonian (with convenient constants inserted),

$$H=2\mathbf{S}\cdot\mathbf{S}'-1/2$$

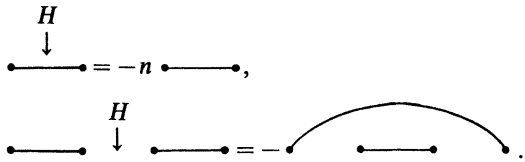
acting on a pair of neighboring spins gives

$$H\psi_\alpha{}^\beta=-\delta_\alpha{}^\beta\psi_\gamma{}^\gamma.$$

Written in this way an obvious generalization from $SU(2)$ to $SU(n)$ suggests itself. The Hamiltonian for the $SU(n)$ model is still defined by the above equation if we allow the indices α to run from 1 to n. The action of H on a valence bond state can be obtained by observing that

$$H\psi_\alpha{}^\alpha=-n\psi_\alpha{}^\alpha \quad \text{and} \quad H_{23}\psi_\alpha{}^\alpha{}_\beta{}^\beta=-\psi_\alpha{}^\beta{}_\beta{}^\alpha.$$

(In the latter equation H_{23} denotes the term in H acting on the second and third sites.) This can be represented graphically as the following:



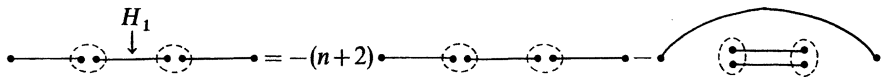
In the $s=1$ case, we again let the indices in the basis vector $\psi_{\alpha\beta}$ run from 1 to n. We now have the symmetric tensor representation $\psi_{\alpha\beta}$ on odd sites and its conjugate representation $\psi^{\alpha\beta}$ on even sites. The Heisenberg Hamiltonian

$$H_1=2\mathbf{S}\cdot\mathbf{S}'-2$$

acting on ψ gives

$$\begin{aligned}H_1\psi_{\alpha_1\alpha_2}{}^{\alpha_3\alpha_4}=&-\delta_{\alpha_1}{}^{\alpha_3}\psi_{\beta\alpha_2}{}^{\beta\alpha_4}-\delta_{\alpha_1}{}^{\alpha_4}\psi_{\beta\alpha_2}{}^{\alpha_3\beta}\\&-\delta_{\alpha_2}{}^{\alpha_3}\psi_{\alpha_1\beta}{}^{\beta\alpha_4}-\delta_{\alpha_2}{}^{\alpha_4}\psi_{\alpha_1\beta}{}^{\alpha_3\beta}.\end{aligned}$$

We may again generalize the Hamiltonian to $SU(n)$ by simply letting the indices run from 1 to n. The action of H_1 on the VBS state can be represented graphically as follows.



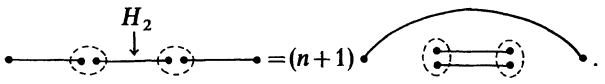
In the $SU(2)$ case the biquadratic Hamiltonian

$$H_2\equiv 2(\mathbf{S}\cdot\mathbf{S}')^2-2$$

produces double bonds on nearest neighbor links

$$H_2\psi_{\alpha\beta}{}^{\gamma\delta}=(\delta_\alpha{}^\gamma\delta_\beta{}^\delta+\delta_\alpha{}^\delta\delta_\beta{}^\gamma)\psi_{\varepsilon\varrho}{}^{\varepsilon\varrho}.$$

Again we extend this definition of H_2 to $SU(n)$. The action on the VBS state can be represented as follows:



Consider the one-dimensional $SU(n)$ quantum "spin" system with "$s=1$" and the general bilinear-biquadratic Hamiltonian

$$H=\sum_i \frac{1}{n}H_1(\mathbf{S}_i,\mathbf{S}_{i+1})-\frac{\beta}{n^2}H_2(\mathbf{S}_i,\mathbf{S}_{i+1}). \tag{4.16}$$

(The factors of n are inserted so that the spacing of eigenvalues of H remains finite as $n\to\infty$.) The $SU(n)$ VBS state introduced in the previous subsection becomes the exact ground state at $\beta=-n/(n+1)$. This can be seen by considering the action of H using the above graphical rules, or by observing that this Hamiltonian is a projection operator onto the $SU(n)$ representation which generalizes $s=1$, namely the symmetrized traceless tensor with two upper and two lower indices. It is worth noting that, in the limit $n\to\infty$, the exact ground states of (4.16) can be constructed entirely out of nearest neighbor valence-bonds for arbitrary β. For $\beta\leqq 0$ the ground state is the VBS state, and for $\beta\geqq 0$ the ground state is the two dimerized states which have double valence-bonds on every other bond. This provides a support for the phase transition picture for the ordinary spin 1 chain described in the introduction and [1].

$SU(n)$ quantum "spin" systems with higher "s" can be defined in a similar way by putting a variable $\psi_{\alpha_1\alpha_2\ldots\alpha_{2s}}$, which transforms under the symmetric $2s$-tensor representation of $SU(n)$, on one sublattice and its conjugate representation $\psi^{\alpha_1\alpha_2\cdots\alpha_{2s}}$ on the other sublattice. When the coordination number z equals $2s$, a Hamiltonian in which the $SU(n)$ VBS state is an exact ground state can be constructed. It is a projection onto the "maximal" representation contained in the product of these two representations, namely the symmetric, traceless tensor with z-upper and z-lower indices.

5. Energy Gap in the Majumdar-Ghosh Model

5.1. The Model and the Ground States

As in Sect. 2, we consider a one-dimensional lattice, but $\mathbf{S}_i$ now denotes the spin operator for spin $s=1/2$ at site i. The Hamiltonian for the Majumdar-Ghosh model is

$$H=\sum_i H_i \quad \text{with } H_i=P_{3/2}(\mathbf{S}_i+\mathbf{S}_{i+1}+\mathbf{S}_{i+2}), \tag{5.1}$$

where $P_{3/2}(\mathbf{S})$ is the orthogonal projection onto the subspace with $\mathbf{S}^2=(3/2)(1+3/2)$ (spin 3/2). This Hamiltonian can be written as the usual spin 1/2 Heisenberg model plus a next nearest neighbor term by using the identity

$$P_{3/2}(\mathbf{S}_i+\mathbf{S}_{i+1}+\mathbf{S}_{i+2})=\tfrac{2}{3}(\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\mathbf{S}_i\cdot\mathbf{S}_{i+2}+\mathbf{S}_{i+1}\cdot\mathbf{S}_{i+2})+\tfrac{1}{2}. \tag{5.2}$$

Valence Bond Ground States in Isotropic Quantum Antiferromagnets

In order to describe the ground states of the system, we again make use of an $SU(2)$ notation similar to that of the previous sections. For a single site we denote the standard $S^3 = \pm 1/2$ basis $\{(+),(-)\}$ by

$$\psi_1 = (+), \quad \psi_2 = (-).$$

We also make use of the raising convention $\psi^\alpha = \varepsilon^{\alpha\beta}\psi_\beta$ and the summation convention for repeated upper and lower indices. For a system on a finite chain $\{1, 2, \ldots, L\}$, we use the basis which consists of simple tensor products of ψ_α's as in Sect. 2. In particular, the following choice is convenient for our purposes.

$$\psi_{\alpha_1}{}^{\alpha_2 \cdots \alpha_{L-1}}{}_{\alpha_L} = \psi_{\alpha_1} \otimes \psi^{\alpha_2} \otimes \ldots \otimes \psi^{\alpha_{L-1}} \otimes \psi_{\alpha_L}. \tag{5.3}$$

Each α_i can be 1 or 2. This equation applies for the case of odd L. If L is even the α_{L-1} should be a lower index and the α_L should be an upper indice. These states provide us with a complete set of states for the finite chain.

The ground states of the Majumdar-Ghosh model are easily written in this notation. For odd L there are four linearly independent ground states given by

$$\begin{aligned} \Omega^{(1)}{}_\alpha &= \psi_{\alpha_1}{}^{\alpha_1}{}_{\alpha_2}{}^{\alpha_2} \cdots {}^{\alpha_{(L-1)/2}}{}_\alpha, \\ \Omega^{(2)}{}_\alpha &= \psi_\alpha{}^{\alpha_1}{}_{\alpha_1}{}^{\alpha_2}{}_{\alpha_2} \cdots {}^{\alpha_{(L-1)/2}}{}_{\alpha_{(L-1)/2}}, \end{aligned} \tag{5.4}$$

with $\alpha = 1$ or 2. For even L there are five linearly independent ground states given by

$$\begin{aligned} \Omega^{(1)} &= \psi_{\alpha_1}{}^{\alpha_1}{}_{\alpha_2}{}^{\alpha_2} \cdots {}^{\alpha_{L/2}}, \\ \Omega^{(2)}{}_\alpha{}^\beta &= \psi_\alpha{}^{\alpha_1}{}_{\alpha_1}{}^{\alpha_2}{}_{\alpha_2} \cdots {}^{\alpha_{(L-2)/2}}{}^\beta, \end{aligned} \tag{5.5}$$

with $\alpha, \beta = 1$ or 2.

As is clear from the formulae, we get two different infinite volume ground states from these states. If we again denote the singlet pairs by line segments, the ground states (5.4) and (5.5) can be represented diagramatically as shown in Fig. 5.1. Unlike the valence-bond solid states, the valence bonds now cover only half of the lattice. Moreover, the ground states have period 2, and thus break the translational symmetry of the Hamiltonian.

Also note that these dimerized ground states are mere tensor products of local singlet pairs. Therefore, correlation functions for these dimerized states are just

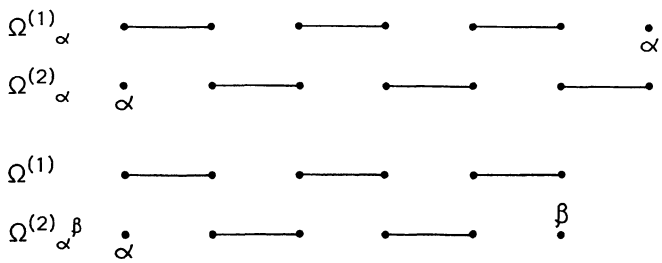


Fig. 5.1. The ground states of the Majumdar-Ghosh model

trivial combinations of singlet pair correlation functions. In particular, the two point correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ vanishes whenever $|i-j| \geqq 2$.

To see that the states in (5.4) and (5.5) are ground states of (5.1), observe that the restriction of each state to any three adjacent sites contains a singlet pair. Therefore, the total spin of these three sites is always 1/2. Then the projection operator representation (5.1) of the Hamiltonian immediately implies that the state has energy zero.

This model and the above states were first discovered by Majumdar and Ghosh [31, 32], and in [15] it was proved that these states were ground states. Some exact excited states were constructed in [19, 39]. For some related results see [40]. We will show that the states in (5.4) and (5.5) are the only ground states and that there is a gap in the spectrum of the Hamiltonian.

5.2. *The Energy Gap*

The techniques used in Sect. 2.3 can also be used to prove there is a gap in the spectrum of the Majumdar-Ghosh Hamiltonian. This subsection is devoted to the existence of the gap in finite chains. The infinite volume result appears at the end of Sect. 5.3.

Theorem 5.1. *Consider the Hamiltonian*

$$H_{1,L} = \sum_{i=1}^{L-2} H_i$$

with H_i defined by (5.1). *There is a positive constant ε which does not depend on L such that*

$$H_{1,L} \geqq \varepsilon P_L ,$$

where P_L is the projection onto the orthogonal complement of the ground states of $H_{1,L}$.

As in Sect. 2 we define Q_n to be the projection onto the subspace of states which are ground states for $H_{1,n}$, and define P_n to be $1-Q_n$. Any ground state for $H_{1,n+1}$ is also a ground state for $H_{1,n}$. Thus the Q_n are a decreasing sequence of projections and the P_n are an increasing sequence of projections. This was the only property of the model that we used in proving Lemmas 2.2 and 2.3 and in using Lemmas 2.2, 2.3, and 2.4 to prove Theorem 2.1. Thus all we have to do in the present case is to prove an analog of Lemma 2.4.

There is one minor difference between Sect. 2.3 and the present model, namely the dimension of $Q_n - Q_{n+1}$. As we will show in Sect. 5.3 the ground states defined by (5.4) and (5.5) are the only ground states. Hence Q_n restricted to sites 1 to n has dimension 5 if n is even and 4 if n is odd. Thus $Q_n - Q_{n+1}$ restricted to sites 1 to $n+1$ has dimension $5 \times 2 - 4 = 6$ if n is even and $4 \times 2 - 5 = 3$ if n is odd. As in Sect. 2 we let φ^i_{n+1} be an orthonormal basis for $Q_n - Q_{n+1}$ on sites 1 to $n+1$ and define $\varepsilon(l)$ as before:

$$\varepsilon(l) = \sup_n \max_i \| Q_{n-l+1,n+1} \varphi^i_{n+1} \|^2 .$$

Valence Bond Ground States in Isotropic Quantum Antiferromagnets

Note that in Sect. 2.3 it would have been sufficient to prove Lemma 2.4 only for even l. Here we will only prove the lemma for even l since it reduces the number of cases we must consider. The analog of Lemma 2.4 is the following.

Lemma 5.2. *There is a constant c such that for all even l*

$$\varepsilon(l) \leqq c 2^{-l/2}. \tag{5.6}$$

Proof. We begin by computing the norms and overlaps of the various ground states. As in Sect. 2 this computation may be done in a diagramatic fashion, but here each calculation only involves one diagram. For example, the overlap of $\Omega^{(1)}{}_{\alpha}$ and $\Omega^{(2)}{}_{\beta}$ is given by the diagram in Fig. 5.2. This diagram simply equals $\delta^{\beta}{}_{\alpha}$. The norm of $\Omega^{(1)}{}_{\alpha}$ is given by a sequence of small loops with one loop for every two sites. Since each loop gives a factor of 2, the square of the norm of $\Omega^{(1)}{}_{\alpha}$ is $2^{(L-1)/2}$. The other norms and overlaps may be computed in the same fashion.

We consider first the case that n is odd. Every state we encounter in the proof will be a ground state for $H_{1,n-l}$ and a ground state for $H_{n-l+1,n}$. Thus it is convenient to introduce the states $\Omega^{(12)}{}_{\alpha\ \gamma}^{\ \beta\ \delta}$, $\Omega^{(21)}{}_{\alpha}^{\ \beta}$, $\Omega^{(11)}{}_{\alpha}^{\ \beta}$, and $\Omega^{(22)}{}_{\alpha\ \gamma}^{\ \beta\ \delta}$ which are defined diagramatically by Fig. 5.3.

Let φ be one of the φ^{i}_{n+1}. Then φ is a ground state of $H_{1,n}$ and so is a linear combination of $\Omega^{(12)}{}_{\alpha\ \gamma}^{\ \alpha\ \delta}$ and $\Omega^{(21)}{}_{\gamma}^{\ \delta}$:

$$\varphi = \Omega^{(12)}{}_{\alpha\ \gamma}^{\ \alpha\ \delta} A^{\gamma}{}_{\delta} + \Omega^{(21)}{}_{\gamma}^{\ \delta} B^{\gamma}{}_{\delta}. \tag{5.7}$$

The norms of the states in Fig. 5.3 are either $2^{(n-1)/4}$ or $2^{(n-3)/4}$. The overlap of $\Omega^{(12)}{}_{\alpha\ \gamma}^{\ \alpha\ \delta}$ and $\Omega^{(21)}{}_{\gamma}^{\ \delta}$ is either 0 or 1. Since φ is defined so that it has norm 1, it follows that

$$|A^{\gamma}{}_{\delta}| = O(2^{-n/4}) \quad \text{for any } \gamma, \delta, \tag{5.8a}$$

$$|B^{\gamma}{}_{\delta}| = O(2^{-n/4}) \quad \text{for any } \gamma, \delta. \tag{5.8b}$$

φ is orthogonal to any state which is a ground state for $H_{1,n+1}$. These ground states include $\Omega^{(12)}{}_{\alpha\ \gamma}^{\ \alpha\ \gamma}$ and $\Omega^{(21)}{}_{\alpha}^{\ \beta}$. We compute their inner products with φ and

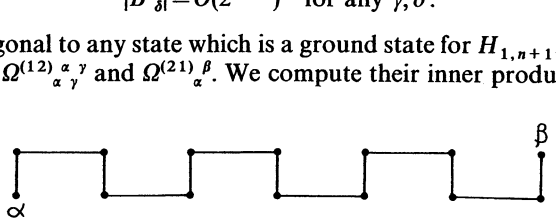


Fig. 5.2. The one diagram which contributes to the overlap of $\Omega^{(1)}{}_{\alpha}$ and $\Omega^{(2)}{}_{\beta}$

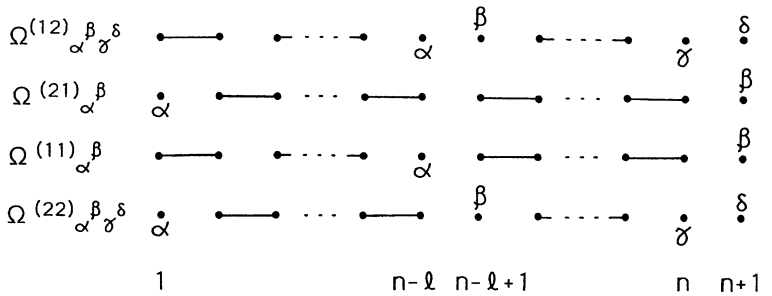


Fig. 5.3. The states which are used in the proof of the existence of a gap

find

$$0=\Omega^{\dagger(21)\gamma}{}_{\delta}\cdot\varphi=A^{\gamma}{}_{\delta}+2^{(n-1)/2}B^{\gamma}{}_{\delta}, \tag{5.9}$$

$$0=\Omega^{\dagger(12)\alpha\ \beta}{}_{\alpha\ \beta}\cdot\varphi=A^{\gamma}{}_{\gamma}2^{(n-1)/2}+B^{\gamma}{}_{\gamma}. \tag{5.10}$$

Equations (5.9) and (5.8a) imply

$$|B^{\gamma}{}_{\delta}|=O(2^{-3n/4}) \quad \text{for any } \gamma,\delta. \tag{5.11}$$

Equations (5.10) and (5.11) imply

$$|A^{\gamma}{}_{\gamma}|=O(2^{-5n/4}). \tag{5.12}$$

Our goal is to show that $\|Q_{n-l+1,n+1}\varphi\|^2$ is $O(2^{-l/2})$. By (5.7) φ is a sum of two terms. The norm of the second term is

$$\|\Omega^{(21)}{}_{\gamma}{}^{\delta}B^{\gamma}{}_{\delta}\|=O(2^{-3n/4})\max_{\gamma,\delta}\|\Omega^{(21)}{}_{\gamma}{}^{\delta}\|=O(2^{-n/2}),$$

where we have used (5.11) and $\|\Omega^{(21)}{}_{\gamma}{}^{\delta}\|=2^{-(n-1)/4}$. Since $n\geqq l$ this implies the square of the norm is $O(2^{-l})$. Thus letting φ' denote the first term in (5.7), i.e., $\varphi'=\Omega^{(12)}{}_{\alpha}{}^{\alpha}{}_{\gamma}{}^{\delta}A^{\gamma}{}_{\delta}$, it suffices to show $\|Q_{n-l+1,n+1}\varphi'\|^2=(\varphi',Q_{n-l+1,n+1}\varphi')$ is $O(2^{-l/2})$.

φ' is a ground state of $H_{1,n-l}$ and $Q_{n-l+1,n+1}$ commutes with this Hamiltonian, so $Q_{n-l+1,n+1}\varphi'$ is a ground state of $H_{1,n-l}$. The vector $Q_{n-l+1,n+1}\varphi'$ is trivially a ground state of $H_{n-l+1,n+1}$, so it is a linear combination of $\Omega^{(12)}{}_{\alpha}{}^{\beta}{}_{\gamma}{}^{\gamma}$, $\Omega^{(21)}{}_{\alpha}{}^{\beta}$, $\Omega^{(11)}{}_{\alpha}{}^{\beta}$, $\Omega^{(22)}{}_{\alpha}{}^{\beta}{}_{\gamma}{}^{\gamma}$. Each of these states has norm $2^{(n-1)/4}$ and their overlaps are 0 or 1. Hence the coefficients in the linear combination must all be $O(2^{-n/4})$. Thus it suffices to show the inner product of φ' with each of these states is $O(2^{-l/2+n/4})$.

The inner product with $\Omega^{(12)}{}_{\alpha}{}^{\beta}{}_{\gamma}{}^{\gamma}$ is $\delta^{\beta}{}_{\alpha}A^{\gamma}{}_{\gamma}2^{(n-3)/2}=O(2^{-3n/4})\leqq O(2^{-l/2+n/4})$ by (5.11). The inner product with $\Omega^{(22)}{}_{\alpha}{}^{\beta}{}_{\gamma}{}^{\gamma}$ also involves $A^{\gamma}{}_{\gamma}$ and is sufficiently small. The inner product with $\Omega^{(11)}{}_{\alpha}{}^{\beta}$ is $A_{\alpha}{}^{\beta}2^{(n-l-1)/2}=O(2^{n/4-l/2})$ by (5.8a). The overlap with $\Omega^{(21)}{}_{\alpha}{}^{\beta}$ is $A_{\alpha}{}^{\beta}=O(2^{-n/4})\leqq O(2^{n/4-l/2})$ since $n\geqq l$.

If n is even the proof is essentially the same. We simply modify Fig. 5.3 by adding a site on the left in an obvious way. □

5.3. *The Infinite Chain*

In this section we show that in the infinite volume limit there are exactly two ground states and each of them has a gap. We denote the four ground states on $\{-L,-L+1,\ldots,L\}$ by $\Omega^{(1,L)}{}_{\alpha}$ and $\Omega^{(2,L)}{}_{\alpha}$, $\alpha=1,2$.

Theorem 5.3. *Let A be a local operator. Then for $i=1,2$, the expectation value*

$$\omega^i(A)=\frac{(\Omega^{(i,L)}{}_{\alpha},A\Omega^{(i,L)}{}_{\alpha})}{(\Omega^{(i,L)}{}_{\alpha},\Omega^{(i,L)}{}_{\alpha})} \quad \textit{(no sum over } \alpha\textit{)} \tag{5.13}$$

is independent of L and α provided that L is large enough that the support of A is contained in the interval $\{-L+1,-L+2,\ldots,L-1\}$. Equation (5.13) *defines two distinct infinite volume ground states ω^1 and ω^2. If ϱ is an infinite volume state which is a ground state in the sense that $\varrho(H_i)=0$ for all i, then $\varrho=c\omega^1+(1-c)\omega^2$ for some constant c, $0\leqq c\leqq 1$.*

The key ingredient in the proof is a finite volume result.

Valence Bond Ground States in Isotropic Quantum Antiferromagnets

Lemma 5.4. *Let φ be a state on $\{-L, -L+1, \ldots, L\}$ which satisfies $H_i\varphi = 0$ for $i = -L, \ldots, L-2$. Then φ can be written as*

$$\varphi = A^\alpha \Omega^{(1,L)}{}_\alpha + B^\alpha \Omega^{(2,L)}{}_\alpha$$

for some complex coefficients A^α and B^α.

Proof of Theorem 5.3. Since the states $\Omega^{(i,L)}{}_\alpha$ are tensor products of states on two sites, the first claim in the theorem is trivial. The states ω^1 and ω^2 are clearly distinct.

Let ϱ be an infinite volume ground state. Choose a local observable B with $\omega^1(B) = 1$ and $\omega^2(B) = 0$, e.g., $B = -(4/3)\mathbf{S}_1 \cdot \mathbf{S}_2$. Let $c = \varrho(B)$. It is easily shown that

$$\lim_{L\to\infty} \frac{(\Omega^{(i,L)}{}_\alpha, A\Omega^{(j,L)}{}_\beta)}{\|\Omega^{(i,L)}{}_\alpha\| \, \|\Omega^{(j,L)}{}_\beta\|} = 0 \tag{5.15}$$

for any local observable A unless $i = j$ and $\alpha = \beta$. Lemma 5.4 and Eq. (5.15) imply $\varrho = c\omega^1 + (1-c)\omega^2$ by an argument similar to the proof of Theorem 2.7. □

Proof of Lemma 5.4. We proceed by induction in the length of the chain. For 3 sites the ground state must be of the form

$$\Omega = \psi_\alpha{}^\alpha{}_\beta A^\beta + \psi_\alpha{}^\beta{}_\beta B^\alpha .$$

(This can be seen by counting dimensions. The above equation yields four linearly independent ground states, and the subspace of total spin 1/2 for the tensor product of three spin 1/2's has dimension four.) For 4 sites any ground state Ω can be written

$$\Omega = \psi_\alpha{}^\alpha{}_\beta{}^\gamma A^\beta{}_\gamma + \psi_\alpha{}^\beta{}_\beta{}^\gamma B^\alpha{}_\gamma ,$$

since it is a ground state for the first three sites, and

$$\Omega = \psi_\alpha{}^\beta{}_\gamma{}^\gamma C^\alpha{}_\beta + \psi_\alpha{}^\beta{}_\beta{}^\gamma D^\alpha{}_\gamma ,$$

since it is a ground state for the last three sites.

We need to show that

$$A^\beta{}_\gamma = C^\beta{}_\gamma = E\delta^\beta{}_\gamma .$$

We again establish these equations by considering various components of Ω. We list the component considered and the corresponding equation.

$\psi_1{}^2{}_2{}^1$: $B^1{}_1 = D^1{}_1$.

$\psi_2{}^1{}_1{}^2$: $B^2{}_2 = D^2{}_2$.

$\psi_1{}^1{}_1{}^1$: $A^1{}_1 + B^1{}_1 = C^1{}_1 + D^1{}_1$.

$\psi_2{}^2{}_2{}^2$: $A^2{}_2 + B^2{}_2 = C^2{}_2 + D^2{}_2$.

$\psi_1{}^1{}_2{}^2$: $A^2{}_2 = C^1{}_1$.

$\psi_1{}^1{}_2{}^1$: $A^2{}_1 = 0$.

$\psi_2{}^2{}_1{}^2$: $A^1{}_2 = 0$.

$\psi_1{}^2{}_1{}^1$: $C^1{}_2 = 0$.

$\psi_2{}^1{}_2{}^2$: $C^2{}_1 = 0$.

The first five equations imply $A^1{}_1 = C^1{}_1 = A^2{}_2 = C^2{}_2$. Thus the most general ground state for 4 sites is

$$\psi_\alpha{}^\alpha{}_\beta{}^\beta E + \psi_\alpha{}^\beta{}_\beta{}^\delta B^\alpha{}_\delta .$$

As in the proof of Lemma 2.8 the general inductive step can be reduced to the above argument. □

We defined the existence of a gap for an infinite volume ground state in Definition 2.11.

Theorem 5.5. *Each of the ground states ω^1 and ω^2 has a gap.*

Proof. Given Theorem 5.1 and Eq. (5.15), the proof is identical to that of Theorem 2.12. □

6. Other Valence Bond Ground States

There exist generalizations of the VBS states of Sects. 2–4 and the dimerized states of Sect. 5 and Hamiltonians for which these states are exact ground states. We present these states and Hamiltonians here. We do not have any general rigorous results, so this section should be viewed primarily as a list of open questions.

The generalized VBS state may be defined for any lattice with coordination number z and spin s at each site provided $s = nz/2$ for some integer n. The generalized VBS state is formed by constructing n valence bonds at each bond in the lattice. We do this by thinking of the spin s at each site as the symmetrization of $2s = nz$ spin 1/2's. For example, this generalized VBS state for the one-dimensional lattice with spin 2 is shown in Fig. 6.1.

A Hamiltonian for which this state is an exact ground state is

$$H = \sum_{(i,j)\in\mathbb{B}} \sum_{s'=2s-n+1}^{2s} a_{s'} P_{s'}(\mathbf{S}_i + \mathbf{S}_j), \tag{6.1}$$

where the $a_{s'}$ are positive constants. The generalized VBS state is a ground state since the restriction of the state to any two adjacent sites contains at least n pairs of spin 1/2's in the singlet state, and so has a total spin of at most $2s-n$. We expect that the nature of the generalized VBS state depends crucially on the dimension, the coordination number and the multiplicity n.

All our rigorous results were for lattices that were bipartite, but we should emphasize that the VBS state and the generalized VBS state can be constructed for lattices which are not bipartite. For example, we may define a VBS state for the triangular lattice with spin 3 at each site. We do not know what properties such a state has, in particular, whether or not the correlation functions decay exponentially.

We can generalize the Majumdar-Ghosh model [31, 32] and some models discovered by Klein [27] as follows. For a lattice with coordination number z and

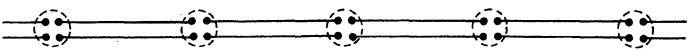


Fig. 6.1. A generalized VBS state

Valence Bond Ground States in Isotropic Quantum Antiferromagnets

spin s at each site let

$$H = \sum_i \sum_{s'=(z-1)s+1}^{(z+1)s} a_{s'} P_{s'}(\mathbf{S}_i + \mathbf{S}_{i_1} + \mathbf{S}_{i_2} + \ldots + \mathbf{S}_{i_z}), \tag{6.2}$$

where $i_1, i_2, \ldots, i_z$ are the nearest neighbors of the site i, and i is summed over the sites in the lattice. Again the $a_{s'}$ are positive constants. Now suppose that we have a state in which every site has $2s$ valence bonds coming out of it and going to some nearest neighbor of that site. (Such states are easily constructed.) Then the restriction of that state to a site i and its z nearest neighbors contains $2s$ valence bonds and so has a maximum spin of $(z+1)s-2s=(z-1)s$. Thus, such a state is a ground state of the above Hamiltonian. For the one-dimensional lattice with spin 1/2 at each site we recover the Majumdar-Ghosh Hamiltonian.

If s is an integral multiple of $z/2$ then the generalized VBS state is a ground state of (6.2). However, the above construction of ground states for (6.2) works even if s is not an integral multiple of $z/2$. In dimensions greater than one this construction of dimerized ground states yields infinitely many infinite volume ground states. For example, with spin $s=1/2$ any covering of the lattice by non-overlapping dimers gives a ground state.

In one dimension, however, we expect that there are only a finite number of ground states for (6.2). For example, some ground states of (6.2) on the one-dimensional lattice with spin 3/2 are shown in Fig. 6.2. We refer to the first two states as fully dimerized and the last two as partially dimerized. In the partially dimerized states any pair of adjacent sites always contains at least one valence bond, and so this pair cannot have total spin 3. Thus a Hamiltonian for which the partially dimerized states are ground states, but the fully dimerized states are not, can be constructed by adding to (6.2) the projections onto spin 3 for each pair of adjacent sites. In the fully dimerized state any two sites which are connected by three valence bonds have a total spin of 0. Thus any three adjacent sites have a total spin of 3/2, and we can form a Hamiltonian for which the fully dimerized states are ground states but the partially dimerized states are not by adding to (6.2) the projection onto spin 1/2 for each group of three adjacent sites. More generally, if we let the sum over s' in (6.2) range over all values except s, then the

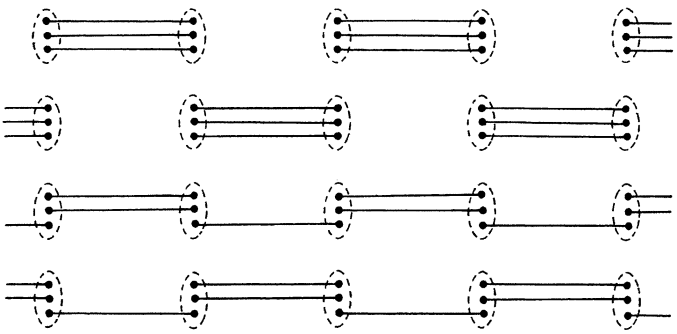


Fig. 6.2. Two fully dimerized ground states and two partially dimerized ground states for the Hamiltonian (6.2)

resulting Hamiltonian will have the fully dimerized states as ground states, and we expect they are the only ground states.

Appendix A. Néel Order in the Hexagonal Lattice Heisenberg Model

In Sect. 3 we showed that in the ground state of a particular Hamiltonian on the two-dimensional hexagonal lattice with spin 3/2 at each site the two-point function has exponential decay, and hence there is no Néel order. This raises the possibility that the usual Heisenberg Hamiltonian on the two-dimensional hexagonal lattice does not have Néel order in its ground state. In this appendix we will use the technique of Gaussian domination to rule out this possibility, i.e., to show that the usual Heisenberg Hamiltonian on this lattice *does* have Néel order provided the spin is at least 3/2.

Gaussian domination was first proven for *classical* spin systems by Fröhlich et al. [22]. Dyson, Lieb, and Simon then proved the property for *quantum* antiferromagnets and used it to show the existence of Néel order at low temperature in the usual Heisenberg antiferromagnet on the cubic lattice for spin $\geqq 1$ in dimension $\geqq 3$ and for spin $\geqq 1/2$ in dimension $\geqq 4$ [21]. In two dimensions there is no Néel order at finite temperature, but for antiferromagnets it is a nontrivial question whether or not there is Néel order in the ground state. Jordão Neves and Fernando Perez [26] observed that the techniques of Dyson, Lieb, and Simon could be used to prove the existence of Néel order in the ground state for two dimensions if the spin is large enough. For the two-dimensional cubic lattice they claimed that the method proved Néel order if the spin is at least 3/2. Unfortunately, there is a mistake in their calculations. The correct version of inequality (9) of [26] should have a 3/2 in place of the 2 inside the square root in the denominator in the left side of this inequality. One then finds that there is Néel order for the two-dimensional square lattice if the spin is at least 1.

Dyson, Lieb, and Simon pointed out in [21] that their proof of Gaussian domination applies to the two-dimensional hexagonal lattice. Thus it is clear that one can show the ground state for this lattice has Néel order if the spin is large enough. Following [21] and [26], it is a routine calculation to show that $s=3/2$ is indeed large enough, so we will only present a few highlights of the calculation.

The only significant difference between the present case and those in [21] and [26] is that we must consider the lattice Laplacian on the hexagonal lattice rather than the usual cubic lattice. This hexagonal lattice Laplacian is defined by

$$(-\Delta\psi)(x)=3\psi(x)-\sum_{y:|x-y|=1}\psi(y), \tag{A.1}$$

where y is summed over the three nearest neighbors of x. To find the eigenvalues and eigenvectors of this operator recall that the two-dimensional hexagonal lattice is bipartite, i.e., it can be written as the disjoint union of two sublattices with any two nearest neighbors belonging to different sublattices. We refer to the sublattices as "even" and "odd."

Let δ_i, $i=1,2,3$ be unit vectors such that for every even site x, the nearest neighbors of x are given by $x+\delta_i$. The nearest neighbors of an odd site y are then given by $y-\delta_i$. For a finite lattice Λ with periodic boundary conditions the

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eigenvalues of $-\Delta$ are then

$$E^{\pm}{}_k = 3 \pm |\varepsilon(k)| \quad \text{with} \quad \varepsilon(k) = \sum_{i=1}^{3} \exp(ik \cdot \delta_i), \tag{A.2}$$

where k ranges over the Brillouin zone for *one* of the two sublattices. The corresponding eigenvectors are

$$h^{\pm}{}_k(x) = (\mp)^x \exp[ik \cdot x + i(-)^x \varphi(k)/2] |\Lambda|^{-1/2}, \tag{A.3}$$

where $(-)^x$ equals $+1$ for even x and -1 for odd x. $(+)^x$ is always $+1$. $\varphi(k)$ is defined by

$$\varepsilon(k) = |\varepsilon(k)| \exp(i\varphi(k)).$$

$|\Lambda|$ denotes the number of sites in the lattice. Note that the number of allowed k's is $|\Lambda|/2$, so that we have the correct number of eigenvalues and eigenvectors.

Following [21] we note that there is a unitary transformation (rotation by π about the 2-axis at each odd site) which sends $S^1{}_x \to (-)S^1{}_x$, $S^2{}_x \to S^2{}_x$, $S^3{}_x \to (-)^x S^3{}_x$. The argument of [21], in particular Lemma 6.1, then proves the Gaussian domination inequality

$$\left(\sum_x (-)^x S^3{}_x \overline{(-\Delta h)(x)}, \sum_y (-)^y S^3{}_y (-\Delta h)(y)\right) \leqq \frac{1}{\beta} \sum_x \overline{h(x)} (-\Delta h)(x), \tag{A.4}$$

where $(\,,\,)$ is the Duhamel two-point function, the bar denotes complex conjugation, and $h(x)$ is any function on the lattice.

Define

$$S^{\pm}{}_k = \sum_x h^{\pm}{}_k(x) S^3{}_x. \tag{A.5}$$

We caution the reader that the $S^{\pm}{}_k$ should not be confused with the raising and lowering operators. $S^{\pm}{}_k$ is a linear combination only of $S^3{}_x$. We now insert one of the eigenvectors $h^{\pm}{}_k$ for h in (A.4). Since $(-)^x h^{\pm}{}_k(x) = h^{\mp}{}_k(x)$, this yields

$$(\overline{S^{\pm}{}_k}, S^{\pm}{}_k) < 1/(\beta E^{\mp}{}_k). \tag{A.6}$$

As in [21], Anderson's lower bound on the ground state energy and some calculation gives an upper bound on the expectation of the double commutator

$$\begin{aligned} \langle [S^{\pm}{}_k, [H, \overline{S^{\pm}{}_k}]] \rangle &\leqq C^{\pm}{}_k, \\ C^{\pm}{}_k &= 2S(S+1/3)E^{\pm}{}_k/3. \end{aligned} \tag{A.7}$$

Following [26], the Gaussian domination inequality (A.6), the Falk-Bruch inequality, the usual sum rule and $\langle S^3{}_x S^3{}_x \rangle = \langle \mathbf{S}_x \cdot \mathbf{S}_x \rangle / 3 = S(S+1)/3$ imply there is Néel order in the ground state if

$$2S(S+1)/3 > \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \sum_{s=-,+} \sum_k [2S(S+1/3)E^{-s}{}_k/(3E^s{}_k)]^{1/2}. \tag{A.8}$$

Define

$$\begin{aligned} I &= \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \sum_{s=-,+} \sum_k [E^{-s}{}_k / E^s{}_k]^{1/2} \\ &= \frac{1}{2|B|} \int_B d^2k \{[E^-{}_k / E^+{}_k]^{1/2} + [E^+{}_k / E^-{}_k]^{1/2}\}, \end{aligned}$$

where B is the Brillouin zone for one of the sublattices and $|B|$ is its area. Then (A.8) becomes

$$(S+1)[2S/(3S+1)]^{1/2} > I. \tag{A.9}$$

For $S=3/2$ the left side is 1.846 ..., and numerical evaluation of the integral yields $I=1.52\pm 0.01$. Thus there is Néel order for spin 3/2 and higher.

Our calculation has been for the two-dimensional hexagonal lattice, but there is an analogous calculation for any bipartite lattice for which Gaussian domination holds. The integral I depends on the lattice type and the dimension, but I is always at least 1 because of the trivial inequality $x+1/x \geqq 2$. As the dimension d increases, I typically decreases to 1. For example, for the cubic lattice $I=1+O(1/d)$ [21]. The coordination number z enters the above calculation only in the bound on the double commutator (A.7). Condition (A.9) then becomes

$$(S+1)[2Sz/3(Sz+1)]^{1/2} > I.$$

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Note added in proof. After the completion of this work we received a preprint [47] by D.P. Arovas, A. Auerbach and F.D.M. Haldane which contains a new representation of the VBS state. Using this representation we have proved some of the conjectures of the present paper including the uniqueness of the infinite volume ground state (and hence the absence of Néel order) for the hexagonal lattice model of Sect. 3. These results are now being prepared for publication.

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Ground State Properties of a Fully Frustrated Quantum Spin System

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We find that ground states of the quantum Heisenberg antiferromagnet on the geometrically frustrated pyrochlore checkerboard lattice are singlets and can be expressed in terms of positive matrices. The magnetization at zero external field vanishes for each frustrated tetrahedral unit separately, and there is an upper bound of 1/8 in natural units on the susceptibility both for the ground state and at finite temperature. These results are the first exact ones in this field and generalize to some other lattices. The approach is also of interest for other spin systems.

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Geometrically frustrated spin systems are known to have many interesting properties that are quite unlike those of conventional magnetic systems or spin glasses [1]. Most results are for classical systems. The first frustrated system, for which the richness of classical ground states was noted, is the triangular lattice [2]. Subsequently, the pyrochlore lattice, which consists of tetrahedra that share sites, was identified as a lattice on which the frustration effects are especially strong [3]. Unusual low-energy properties, in particular the absence of ordering at any temperature, were predicted for both discrete [3] and continuous [4] classical spin systems. The ground state and low-energy properties of the classical pyrochlore antiferromagnet—whose quantum version is the focus of this Letter—has been extensively studied in [5]. Both the interest and difficulty in studying frustrated spin systems stem from the large ground state degeneracy, which precludes most perturbative approaches.

As is the case for most other strong interacting systems in more than one dimension, very little is known exactly about the ground states of frustrated quantum spin systems. Most of the present knowledge has been obtained by numerics or clever approximations. Quantum fluctuations have been studied in the limits of large S [6], where a tendency towards lifting the ground state degeneracy in favor of an ordered state ("quantum order by disorder") was detected. In the opposite limit, $S = 1/2$, where quantum fluctuations are much stronger, the pyrochlore antiferromagnet has been identified as a candidate for a quantum disordered magnet ("quantum spin liquid") [7], and it has also been discussed in terms of a resonating valence bond approach [8]. However, there are no exact results against which to test the reliability of the results in this limit. In contrast to this, for conventional—bipartite—antiferromagnetic spin systems it is well known, for example, that the energy levels are ordered in a natural way according to spin, starting from spin zero [9]. Geometrically frustrated systems are not bipartite and thus this otherwise quite general theorem does not apply.

In this Letter, we find some first exact results for the fully frustrated quantum antiferromagnet on a pyrochlore checkerboard, with the help of the reflection symmetry of this two dimensional lattice. We shall establish rigorously that there is always a ground state with total spin zero. Furthermore, in the periodic case all ground states (if there is more than one) have total spin zero, the spin expectation vanishes for each frustrated unit (this is the quantum analog of the *ice rule* for the Ising system), and there are concrete upper bounds on the susceptibility.

Geometric frustration occurs typically for spin systems with interactions that favor antialignment and involve fully connected units of three or more spins that can obviously not all be mutually antialigned. The kagome lattice is an example of frustrated spin systems with site-sharing triangular units; the pyrochlore lattice and its two-dimensional version, the pyrochlore checkerboard, are examples with site-sharing tetrahedra. We shall focus on the latter; it is a two-dimensional array of site-sharing tetrahedra, whose projection onto a plane is a square lattice with two extra diagonal bonds on every other square. (The regular pyrochlore lattice is a three-dimensional array of site-sharing tetrahedra.) The tetrahedra, or squares with extra diagonal bonds, are the frustrated units and will henceforth be called *boxes*.

The Hamiltonian of a quantum Heisenberg antiferromagnet on a general lattice is (in natural units)

$$H_{\mathrm{AF}} = \sum_{\langle i,j \rangle} \mathbf{s_i} \cdot \mathbf{s_j}, \tag{1}$$

where the sum is over bonds $\langle i, j \rangle$ that connect sites i and j and $\mathbf{s} = (s^1, s^2, s^3)$ are spin operators in the

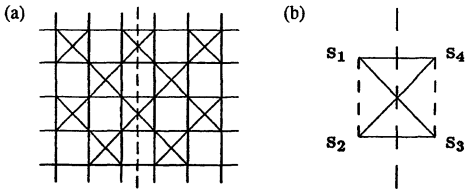

FIG. 1. (a) Pyrochlore checkerboard, reflection symmetric about dashed line; (b) frustrated unit with crossing bonds.

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spin-s representation, where s can be anything. For the checkerboard lattice the Hamiltonian is up to a constant equal to half the sum of the total spin squared of all boxes (labeled by x),

$$H = \frac{1}{2}\sum_x (\mathbf{s}_1 + \mathbf{s}_2 + \mathbf{s}_3 + \mathbf{s}_4)_x^2 . \qquad (2)$$

A 3×3 checkerboard with periodic boundary conditions, i.e., with four independent sites, provides the simplest example. It has a Hamiltonian that is (up to a constant) the total spin squared of one box, and the energy levels, degeneracies, and eigenstates follow from the decomposition of the Hilbert space of four spin-s particles into components of total spin; all ground states have total spin zero, and there are $2s + 1$ of them.

A checkerboard lattice of arbitrary size, with or without periodic boundary conditions but with an even number of independent sites, has the property that it can be split into two equal parts that are mirror images of one another about a line that cuts bonds, as indicated in Fig. 1, and that contains no sites. We shall now show that such a system has at least one spin-zero ground state. It is actually not important, for the following argument, what the lattice looks like on the left or right; these sublattices neither need to be checkerboards nor do they have to be purely antiferromagnetic (as long as total spin is a good quantum number). What is important is that the whole system is reflection symmetric about the line that separates left and right and that the crossing bonds are of checkerboard type. [For a system with periodic boundary conditions (PBCs) in one direction there will actually be two such lines, but we emphasize that PBC is not needed here even though it is needed in the usual reflection positivity applications; see [10] and references therein.] A key observation is that these crossing bonds [solid lines in Fig. 1(b)] form antiferromagnetic bonds $\mathbf{S_L} \cdot \mathbf{S_R}$ between pairs of spins $\mathbf{S_L} = \mathbf{s}_1 + \mathbf{s}_2$ and $\mathbf{S_R} = \mathbf{s}_3 + \mathbf{s}_4$ of each box on the symmetry line.

The Hamiltonian is $H = H_L + H_R + H_C$, where H_L and H_R act solely in the Hilbert spaces of the left and right, respectively, subsystems and H_C contains the crossing bonds. For the checkerboard $H_C = \sum_y [(\mathbf{s}_1 + \mathbf{s}_2) \cdot (\mathbf{s}_3 + \mathbf{s}_4)]_y$, with the sum over boxes y that are bisected by the symmetry line. H_L and H_R are completely arbitrary as long as they commute with the total spin operator. We will, however, assume here that they are real in the S^3 basis. Any state of the system can be written in terms of a matrix c as

$$\psi = \sum_{\alpha,\beta} c_{\alpha\beta}\psi_\alpha^L \otimes (\psi_\beta^R)_{\text{rot}} , \qquad (3)$$

where the ψ_α^L form a real orthonormal basis of S^3 eigenstates for the left subsystem and the $(\psi_\beta^R)_{\text{rot}}$ are the corresponding states for the right subsystem, but rotated by an angle π around the 2 direction in spin space. This rotation takes $\uparrow$ into $\downarrow$, $\downarrow$ into $-\uparrow$, and more generally $|s,m\rangle$ into $(-)^{s-m}|s,-m\rangle$. It reverses the signs of the operators S^1 and S^3, while it keeps S^2 unchanged. The eigenvalue problem $H\psi = E\psi$ is now a matrix equation

$$h_L c + c(h_R)^T - \sum_{i=1}^{3}\sum_y t_y^{(i)} c (t_y^{(i)})^T = Ec , \qquad (4)$$

where $(h_L)_{\alpha\beta}$ and $(h_R)_{\alpha\beta}$ are real, symmetric matrix elements of the corresponding terms in the Hamiltonian and the $t_y^{(i)}$ are the *real* matrices defined for the spin operators $\mathbf{s}_1$ and $\mathbf{s}_2$ in box y by $t_{\alpha\beta}^{(1,3)} = \langle\psi_\alpha^L|s_1^{(1,3)} + s_2^{(1,3)}|\psi_\beta^L\rangle$ and $t_{\alpha\beta}^{(2)} = i\langle\psi_\alpha^L|s_1^{(2)} + s_2^{(2)}|\psi_\beta^L\rangle$. Note the overall minus sign of the crossing term in (4): replacing $\mathbf{s}_1 + \mathbf{s}_2$ by $\mathbf{s}_3 + \mathbf{s}_4$ and ψ^L by $(\psi^R)_{\text{rot}}$ gives a change of sign for directions 1 and 3, while the i in the definition of $t^{(2)}$ gives the minus sign for direction 2.

Consider now the energy expectation in terms of c:

$$\langle\psi|H|\psi\rangle = \text{tr} cc^\dagger h_L + \text{tr} c^\dagger c h_R - \sum_{i,y} \text{tr} c^\dagger t_y^{(i)} c (t_y^{(i)})^\dagger . \qquad (5)$$

Since H is left-right symmetric and by assumption real, we find that for an eigenstate of H with coefficient matrix c there is also an eigenstate with matrix $c^\dagger$ and, by linearity, with $c + c^\dagger$ and $i(c - c^\dagger)$. Without loss of generality we may, therefore, write eigenstates of H in terms of Hermitian $c = c^\dagger$. We shall also take ψ to be normalized: $\langle\psi|\psi\rangle = \text{tr} c^\dagger c = 1$. Following [11], let us write the trace in the last term of (5) in the diagonal basis of c: $-\text{tr} c^\dagger t_y^{(i)} c (t_y^{(i)})^\dagger = -\sum_{k,l} c_k c_l |(t_y^{(i)})_{kl}|^2$. This expression clearly does not increase if we replace all the c_k by their absolute values $|c_k|$, i.e., if we replace the matrix c by the positive semidefinite matrix $|c| = \sqrt{c^2}$. The first two terms in (5) and the norm of ψ remain unchanged under this operation. We conclude that if c is a ground state then so is $|c|$. Since $c = c^+ - c^-$ and $|c| = c^+ + c^-$, with positive semidefinite (p.s.d.) c^+ and c^-, we may, in fact, choose a basis of ground states with p.s.d. coefficient matrices.

Next, we show that the state ψ_0 with the unit matrix as coefficient matrix (in the S^3 eigenbasis) has total spin zero. Since the overlap of ψ_0 with a state with matrix c is simply the trace of c, which is necessarily nonzero for states with a p.s.d. matrix, and because spin is a good quantum number of the problem, this will imply that there is at least one ground state with total spin zero. First consider a spin-1/2 system. In the S^3 eigenbasis every site has then either spin up or spin down. The state with unit coefficient matrix is a tensor product of singlets on corresponding pairs of sites $i \in L$, $i' \in R$ of the two sublattices:

$$\psi_0 = \bigotimes_{i\in L} [\uparrow (\uparrow)_{\text{rot}} + \downarrow (\downarrow)_{\text{rot}}]_{ii'} = \bigotimes_{i\in L} (\uparrow\downarrow - \downarrow\uparrow)_{ii'} . \qquad (6)$$

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The analogous state for a system with arbitrary spins,

$$\psi_0 = \bigotimes_{i\in L} \sum_{m=-s}^{s} [(-)^{s-m}|s,m\rangle \otimes |s,-m\rangle]_{ii'}, \quad (7)$$

is also a tensor product of spin-zero states.

Finally, we show that the projection onto the spin-zero part of a state with p.s.d. coefficient matrix preserves its positivity. This is only of academic interest here, but it is nontrivial and may very well be important for other physical questions. To find the projection onto spin zero we need to decompose the whole Hilbert space into tensor products of the spin components $[j]_k \otimes [j']_{k'}$ of the two subsystems; here k, k' are additional quantum numbers that distinguish multiple multiplets with the same spin j. Only tensor products with $j = j'$ can have a spin-zero subspace, which is unique, in fact, and generated by the spin-zero state $\sum_{m=-j}^{j} |j,m,k\rangle \otimes (-)^{j-m}|j,-m,k'\rangle$. Noting that $(-)^{j-m}|j,-m,k'\rangle$ is precisely the spin-rotated state $(|j,m,k'\rangle)_{\rm rot}$, we convince ourselves that the projection onto spin zero amounts to a partial trace over m in a suitably parametrized matrix c. This operation preserves positive semidefiniteness, so we actually proved that the checkerboard has at least one ground state that has both total spin zero *and* a p.s.d. coefficient matrix c.

We do not know how many ground states there are. To determine the spin of any remaining ground states we add an external field to the Hamiltonian and study the resulting magnetization. We see that the spontaneous magnetization of every box on the symmetry line vanishes for all ground states, and thus, if we have periodic boundary conditions in at least one direction, the total magnetization vanishes. Since $S^3_{\rm tot}$ is a good quantum number and $S^{\pm}_{\rm tot}$ commute with the Hamiltonian, this will imply that all ground states in such a system have total spin zero. Let us thus modify the original Hamiltonian (2) by replacing the term $(s_1^{(3)} + s_2^{(3)} + s_3^{(3)} + s_4^{(3)})_z^2$ for a single box, z, on the symmetry line by $(s_1^{(3)} + s_2^{(3)} + s_3^{(3)} + s_4^{(3)} - b)_z^2$, i.e., effectively adding a field b to the spins in box z and a constant term $\frac{1}{2}b^2$ to the Hamiltonian. We want to distribute the resulting b terms $(s_1^{(3)} + s_2^{(3)} - b/2)^2$, $(s_3^{(3)} + s_4^{(3)} - b/2)^2$, and $2(s_1^{(3)} + s_2^{(3)} - b/2)(s_3^{(3)} + s_4^{(3)} - b/2)$ to H_L, H_R, H_C, respectively. We cannot use the spin rotation as before, because the crossing terms in the Hamiltonian would no longer be left-right symmetric in the basis (3). To avoid this problem we will, instead, expand eigenstates ψ in the same basis on the left and on the right:

$$\psi = \sum_{\alpha,\beta} \tilde{c}_{\alpha\beta} \psi^L_\alpha \otimes \psi^R_\beta . \quad (8)$$

In this basis the Hamiltonian is left-right symmetric and we may assume, as before, that $\tilde{c} = \tilde{c}^\dagger$. Except for the presence of b in box z the energy expectations on the left and right are as before. The energy expectation of the crossing terms of box z in the diagonal basis of $\tilde{c}$ is now

$$\sum_{k,l} \tilde{c}_k \tilde{c}_l [|(t_z^{(1)})_{kl}|^2 - |(t_z^{(2)})_{kl}|^2 + |(t_z^{(3)})_{kl} - b/2|^2] .$$

This expression clearly does not increase if we replace the c_k by their absolute value $|c_k|$ *and* change the signs of the first and last terms. The sign change can be achieved by simultaneously performing a spin rotation and changing the sign of the field b in the right subsystem. This actually completely removes b from the Hamiltonian. We have thus shown that the ground state energies of the systems H_b with and H_0 without the b terms satisfy the inequality $E_b \geq E_0$. Let $|b\rangle$ be a ground state of H_b and $|0\rangle$ a ground state of H_0. It follows from the variational principle that $\langle 0|H_b|0\rangle \geq \langle b|H_b|b\rangle = E_b \geq E_0$. Expressed in terms of spin operators, this reads $E_0 - 2\langle 0|b(s_1^{(3)} + s_2^{(3)} + s_3^{(3)} + s_4^{(3)})_z|0\rangle + b^2 \geq E_0$. Recalling that we are free to choose both the sign and the magnitude of b we find that the ground state magnetization of box z must be zero:

$$\langle 0|(s_1^{(3)} + s_2^{(3)} + s_3^{(3)} + s_4^{(3)})_z|0\rangle = 0 . \quad (9)$$

This quantum analog of the *ice rule* is true for any box on the symmetry line, and it holds for all three spin components. In a system with periodic boundary conditions and an even number of sites in at least one direction we can choose the symmetry line(s) to intersect any given box, so in such a system the magnetization is zero both for every single box separately and also for the whole system: $\langle 0|S^{(3)}_{\rm tot}|0\rangle = 0$. As mentioned previously, this implies that the total spin is zero for all ground states of such a system.

Let us return to the inequality $E_b \geq E_0$. It implies a bound on the local susceptibility of the system: Let $E(b) \equiv \langle b|H_0 - bS^{(3)}_{\rm box}|b\rangle$ be the ground state energy of the periodic pyrochlore checkerboard with a single box immersed in an external field b. Recalling $H_b = H_0 - bS^{(3)}_{\rm box} + \frac{1}{2}b^2$, we see that the above inequality becomes $E(b) + \frac{1}{2}b^2 \geq E(0)$ and, assuming differentiability, implies an upper bound on the susceptibility at zero field for single-box magnetization,

$$\chi_{\rm loc} = -\frac{1}{\lambda}\frac{\partial^2 E(b)}{\partial b^2}\bigg|_{b=0} \leq \frac{1}{4}, \quad (10)$$

where $\lambda = 4$ is the number of spins in a box. (The susceptibility is given in natural units in which we have absorbed the g factor and Bohr magneton in the definition of the field b.)

We would like to get more detailed information about the response of the spin system to a global field $\{b_x\}$ in a Hamiltonian $H_{\{b_x\}}$ which is identical to (2), except for the terms for the third spin component, which are replaced by $(s_1^{(3)} + s_2^{(3)} + s_3^{(3)} + s_4^{(3)} - b_x)_x^2$. From what

we have seen so far, it is apparent that the corresponding ground state energy $E_{\{b_x\}}$ is extremal for $b_x = 0$. With the help of a more sophisticated trace inequality [12] that becomes relevant whenever the matrix c in (3) cannot be diagonalized, one can actually show that $E_{\{b_x\}}$ has an absolute minimum at $b_x = 0$:

$$E_{\{b_x\}} \geq E_0 . \tag{11}$$

Note that we had to put the field on the boxes for this result to hold; not every field on the individual spins can be written this way. The special choice $b_x = B/2$ corresponds to a global homogeneous field B on all spins. (The factor $1/2$ adjusts for the fact that every spin is shared by two boxes.) If $E(B) = \langle B|H_0 - BS^{(3)}_{\rm tot}|B\rangle$ is the ground state energy of the periodic pyrochlore checkerboard in the external field B, then (11) implies $E(B) + \frac{\Lambda}{16}B^2 \geq E(0)$, and thus an upper bound on the susceptibility per site at zero field (in natural units)

$$\chi = -\frac{1}{\Lambda}\frac{\partial^2 E(B)}{\partial B^2}\bigg|_{B=0} \leq \frac{1}{8}, \tag{12}$$

where Λ is the number of independent sites, which equals twice the number of boxes.

All these results continue to hold at finite temperature. The analog of (11) holds also for the partition function corresponding to $H_{\{b_x\}}$,

$$Z_{\{b_x\}} \leq Z_0 , \tag{13}$$

as can be shown by a straightforward application of lemma 4.1 in section 4 of [10] to the pyrochlore checkerboard. The physically relevant partition function for the periodic pyrochlore checkerboard at finite temperature in a homogenous external field, $Z(B) \equiv {\rm tr} e^{-\beta(H_0 - BS^{(3)}_{\rm tot})}$, differs from $Z_{\{b_x\}}$, where $b_x = B/2$, only by a factor corresponding to the constant term in $H_{\{b_x\}}$. Because of (13), the free energy $F(B) = -\beta^{-1}\ln Z(B)$ satisfies

$$F(B) + \frac{\Lambda}{16}B^2 \geq F(0) . \tag{14}$$

This implies (i) that the magnetization at zero field is still zero at finite temperature,

$$M_T = -\frac{1}{\Lambda}\frac{\partial F(B)}{\partial B}\bigg|_{B=0} = 0, \tag{15}$$

and, more interestingly, (ii) the same upper bound for the susceptibility per site at zero field as we had for the ground state,

$$\chi_T = -\frac{1}{\Lambda}\frac{\partial^2 F(B)}{\partial B^2}\bigg|_{B=0} \leq \frac{1}{8} . \tag{16}$$

The bounds on the susceptibility hold for arbitrary intrinsic spin s and agree very well with the results of [13] for the classical pyrochlore antiferromagnet in the undiluted case.

It is not essential for our method that only every other square of the pyrochlore checkerboard is a frustrated unit; only the reflection symmmetry and the antiferromagnetic crossing bonds are important. We could, e.g., have diagonal bonds on *every* square, but then the horizontal and/or vertical bonds must have twice the coupling strength. Our results also apply to various three-dimensional cubic versions of the checkerboard, e.g., with diagonal crossing bonds in every other cube. While the method does not directly work for the 3D pyrochlore lattice because its geometry is too complicated, it has been seen in [5] that classically this system has similar properties to the pyrochlore checkerboard, which is also fully frustrated, and has the added advantage of being more easily visualized.

We thank Roderich Moessner for bringing this problem to our attention, for explaining his work on the classical pyrochlore antiferromagnet, and for numerous helpful discussions and suggestions.

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Part VII

The Polaron

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Exact Ground State Energy of the Strong-Coupling Polaron*

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Dedicated to the memory of R.L. Dobrushin and P.W. Kasteleyn, two founders of modern statistical mechanics

Abstract: The polaron has been of interest in condensed matter theory and field theory for about half a century, especially the limit of large coupling constant, α. It was not until 1983, however, that a proof of the asymptotic formula for the ground state energy was finally given by using difficult arguments involving the large deviation theory of path integrals. Here we derive the same asymptotic result, $E_0 \sim -C\alpha^2$, and with explicit error bounds, by simple, rigorous methods applied directly to the Hamiltonian. Our method is easily generalizable to other settings, e.g., the excitonic and magnetic polarons.

The polaron Hamiltonian of Fröhlich [1] is a model for the Coulomb interaction of one or more electrons with the quantized phonons of an ionic crystal. In the course of time it was also seen to be an interesting field theory model of non-relativistic particles interacting with a scalar boson field, and it was widely studied [2–9] in both contexts.

The model has one dimensionless coupling constant, α, and it was noticed very early that there seems to be a qualitative difference in the ground state between the weak coupling regime, well described by perturbation theory [8], in which the electron is spread out, and the strong coupling regime in which the electron appears to be trapped in a phonon hole of its own making. (This question of trapping seems to have first been considered by Landau [10] in the context of a classical phonon field.)

By now it seems doubtful that such a trapping actually occurs [7, 11, 12], but it remains true that the calculation of the ground state energy, $E_0(\alpha)$, is very different in the two regimes. The strong coupling theory was studied by Pekar [2] (see also [3–5, 9]) who hypothesized that in this limit the total ground state wave function Ψ could be taken to be a product of an electronic function $\phi(x)$ and a phonon function $|\xi\rangle$. It is a fact that this ansatz, called the adiabatic approximation, yields exactly the same result for the ground state energy as the corresponding model with classical phonons. This

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stems from the fact that the phonon operators enter only linearly and quadratically in the Hamiltonian.

Fröhlich's Hamiltonian in appropriate units is

$$H = \mathbf{p}^2 + \sum_{\mathbf{k}} a_{\mathbf{k}}^* a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2} \sum_{\mathbf{k}} \left[\frac{a_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + h.c. \right], \tag{1}$$

where $\mathbf{p} = -i\nabla$ is the electron momentum operator, $\mathbf{x}$ is its coordinate, and V is the volume of the crystal, which tends to infinity. The $\mathbf{k}$'s are the usual normal modes (e.g., $\mathbf{k} = 2\pi V^{-1/3}(n_1, n_2, n_3)$ for a cubic box) and, as usual, $V^{-1}\sum_{\mathbf{k}} \to (2\pi)^{-3}\int d^3k$. Also, as usual, the $\mathbf{k} = 0$ mode is omitted. When $\langle\Psi|H|\Psi\rangle$ is computed with Pekar's ansatz one easily finds that the phonon part $|\xi\rangle$ can be easily evaluated by "completing the square" and the resulting ϕ minimizes the energy

$$\mathcal{E}(\phi) \equiv \int |\nabla\phi|^2 d^3x - \alpha \int\int \frac{\phi(\mathbf{x})^2\phi(\mathbf{y})^2}{|\mathbf{x}-\mathbf{y}|} d^3x d^3y \tag{2}$$

subject to $\int \phi(\mathbf{x})^2 d^3x = 1$. This, as we mentioned above, is what one would get if the $a_{\mathbf{k}}$'s are replaced by c-numbers $\xi_{\mathbf{k}}$.

It has been proved [13] that there is exactly one ϕ, up to translations, that minimizes $\mathcal{E}(\phi)$. By scaling, the minimum energy (call it $E_P(\alpha)$) is proportional to $-\alpha^2$. The question we address is this: *Is this energy, $E_P(\alpha)$, asymptotically exact as α tends to infinity?* Since it is given by a variational calculation, $E_P(\alpha)$ is an upper bound to $E_0(\alpha)$; the problem is to find a lower bound that agrees with $E_P(\alpha)$ to leading order. *We provide such a lower bound in (31) below.*

For a long time more or less the only thing that could be done to validate $E_P(\alpha)$ rigorously was a lower bound [14] of the right order, $-\alpha^2$, but which was about a factor of 3 too large. It was not until 1983, with a precursor in [15], that a complete proof of the asymptotic correctness of $E_P(\alpha)$ was given by Donsker and Varadhan [16]. The proof starts with a familiar expression for the ground state energy,

$$E_0(\alpha) = \lim_{\beta\to\infty} \frac{1}{\beta} \ln\langle\Psi|e^{-\beta H}|\Psi\rangle, \tag{3}$$

with Ψ such that its spectral resolution contains the ground state energy or low energy spectrum of H but is otherwise arbitrary. Now in fact there is a relatively simple Feynman-Kac formula for the semigroup $e^{-\beta H}$ first noted by Feynman in [18]; by integrating out the phonon coordinates in this formula, one finds that the right side of (3) can be replaced by the expression

$$\lim_{\beta\to\infty} \frac{1}{\beta} \ln E \left\{ \exp(\alpha \int_0^\beta \int_0^s \frac{e^{-(t-s)}}{|\mathbf{x}(t)-\mathbf{x}(s)|} ds dt) \right\}. \tag{4}$$

Here, E represents path space expectation for the Brownian motion $\mathbf{x}(t)$. The Feynman-Kac formula and functional integral are discussed in some detail by Ginibre [19] and Roepstorff [20].

It is this limit (4) that Donsker and Varadhan analyze, in effect showing that the Pekar functional (2) provides a kind of large deviation rate function for the functional integral in (4). Their proof is very far from simple and requires an enormous knowledge of large deviation theory of Brownian motion, a subject unknown to most physicists, and it does not generalize easily to other models. Owing to the double integral in (4)

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it is necessary to construct a large deviation theory for "infinitely many variables". Moreover, no error bounds were provided [17]. We note that previously Feynman had used this formula to estimate the ground state energy from above, but his estimate is not sharp even for $\alpha \to \infty$. See also [21] where this functional integral is again employed to obtain a lower bound on the ground state energy which, however, is not sharp.

Regarding the matter of error bounds, we note that Gross [5] takes advantage of momentum conservation to eliminate three phonon degrees of freedom and transforms the Hamiltonian H to a new form involving a sum of α^2-, α^0- and α^{-2}-terms. (He continues to employ the Pekar ansatz.) This form of the Hamiltonian perhaps suggests that the ground state energy itself has an asymptotic expansion in inverse powers of α^2. But the terms in this transformed Hamiltonian are unbounded operators, and so the order of their contributions to the energy is by no means obvious. The bound we obtain on the error is actually $O(\alpha^{9/5})$, which is to be compared with the main term $O(\alpha^2)$.

In any event, there is the following problem: The Pekar ansatz is based on the physically appealing notion that at large coupling the phonons cannot follow the rapidly moving electron (as they do at weak coupling) and so resign themselves to interacting only with the "mean" electronic density, $\phi(\mathbf{x})^2$. What, exactly, do these somewhat anthropomorphic words mean? If they are so very physical, they should be quantifiable and it should not take four decades to build a proof of their correctness. Moreover, one should be able to find a proof that is relatively simple (since the idea is a simple one), and one that also yields some kind of quantitative error estimate. It should also be robust enough to allow an easy extension to some variations of H, such as having several electrons instead of one (the polaronic exciton), inclusion of magnetic fields, an electron kinetic energy, $T(\mathbf{p})$, other than $\mathbf{p}^2$ (for which the semigroup $\exp[-T(\mathbf{p})]$ might not even have a positive kernel), accommodation of $\mathbf{k}$-dependence and nonlinearity in the phonon self energies, electron-phonon interaction energies other than $1/|\mathbf{k}|$, etc.

The method presented here satisfies, we believe, the criteria of simplicity, robustness and, of course, rigor. For this reason it might be of general interest in condensed matter theory or field theory. Despite its generality we shall, for clarity, restrict our discussion to the original Hamiltonian, H.

Before going into the details, it is helpful to give an overview of our method. The first thing to notice is that Pekar's ansatz amounts, mathematically, to saying that we can replace the operators $a_{\mathbf{k}}$ by c-numbers $\xi_{\mathbf{k}}$. One might think, at first, that such a replacement always leads to a lower bound for the energy, but this is false. (If it were true, the small α energy would have to be proportional to $-\alpha^2$ instead of the much more negative, correct value $-\alpha$.) To pursue this idea, nevertheless, the natural tool to think of is coherent states for each phonon mode $\mathbf{k}$. As is well known, these states are indexed by complex numbers $\xi = p + iq$ and, if $|\xi\rangle\langle\xi|$ is the projector onto the coherent state $|\xi\rangle$, we have that

$$\int |\xi\rangle\langle\xi| \, d\xi d\xi^* = I, \tag{5}$$

$$\int \xi \, |\xi\rangle\langle\xi| \, d\xi d\xi^* = a, \tag{6}$$

and

$$\int (|\xi|^2 - 1)|\xi\rangle\langle\xi| \, d\xi d\xi^* = a^* a. \tag{7}$$

It is the extra term -1 *in the last integral that kills the lower bound and gives an unwanted energy* -1 *for each phonon mode* (and hence a negative contribution to the energy that is infinite both because there is no infrared and no ultraviolet cutoff). In other

words, coherent states would give us what we want (effectively replacing the operator a by the number ξ), were it not for the unfortunate fact that the positive *operator* a^*a is represented by the nonpositive *symbol*, $|\xi|^2 - 1$.

Our remedy will be to reduce the effective number of phonon modes to a *finite* number of $O(\alpha^{9/5})$, independent of V. This will not sacrifice rigor because we shall prove that the reduction affects the energy only to $O(\alpha^{9/5})$ at most. These modes will be quite different from the original $a_{\mathbf{k}}$ modes; indeed they will be the $a_{\mathbf{k}}$ modes summed over boxes in $\mathbf{k}$-space of size $\alpha^{3/5}$. Thus, our physical description of strong coupling will be a little different from the conventional one. *Instead of saying that the phonons cannot follow the electron, our point of view will be that the electron significantly excites only finitely many field modes.*

This mode reduction is accomplished in several steps which can be outlined as follows.

• **I.** Using a simple commutator estimate (as in Schrödinger's elementary proof of Heisenberg's uncertainty principle [22]) we can show that $|\mathbf{k}|$ values larger than $K \approx \alpha^{6/5}$ can be ignored with an energy cost of only $\alpha^{9/5}$. This eliminates the ultraviolet problem, i.e., the fact that $|\mathbf{k}|^{-2}$ is not summable.

• **II.** With the same energy error we can localize the electron to a cube of side length $\alpha^{-9/10}$.

• **III.** We decompose the ball $|\mathbf{k}| < K$ into blocks of size $\alpha^{3/5}$, each containing n $\mathbf{k}$-values (with $n \sim V\alpha^{9/5}$). There are about $\alpha^{9/5}$ blocks. Because the electron coordinate $\mathbf{x}$ has been localized, the function $\exp(i\mathbf{k} \cdot \mathbf{x})$ in H can be replaced, in a block B, by $\exp(i\mathbf{k}_B \cdot \mathbf{x})$, where $\mathbf{k}_B$ is any conveniently chosen point in B; the energy penalty is again $\alpha^{9/5}$. The effect of this decoupling is that the electron interacts only with the one mode $A_B \approx n^{-1/2} \sum_{\mathbf{k} \in B} a_{\mathbf{k}}$, from block B. Thus, the electron ends up interacting with only $\alpha^{9/5}$ modes , which is a finite number!

• **IV.** These active modes can now be represented by coherent state integrals, as above. The unwanted -1 term now contributes only $\alpha^{9/5}$ to E_0, that being the number of modes.

The details will now be given.

I. We first establish a commutator inequality which will show that the large $\mathbf{k}$ modes of the Hamiltonian may be discarded at the price of only a small decrease in the coefficient of the $\mathbf{p}^2$ term of the Hamiltonian. For any normalized state with expectation $\langle \cdot \rangle$, we have

$$\begin{aligned} |k_j| \, |\langle a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \rangle| &= |\langle [p_j, a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}] \rangle| \\ &\leq 2 \langle p_j^2 \rangle^{1/2} \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle^{1/2} \end{aligned} \tag{8}$$

for each phonon momentum coordinate k_j, $j = 1, 2, 3$, just by the Schwarz inequality. Squaring this inequality, summing over j, and then taking the square root, we obtain

$$|\langle a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \rangle| \leq \frac{2}{|\mathbf{k}|} \langle \mathbf{p}^2 \rangle^{1/2} \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle^{1/2}. \tag{9}$$

A similar inequality holds for $a_{\mathbf{k}}$ replaced by $a_{\mathbf{k}}^*$. It follows that for any $\varepsilon > 0$, and with $K \equiv 8\alpha/\pi\varepsilon$,

$$
\begin{aligned}
&-(\frac{4\pi\alpha}{V})^{1/2}\sum_{|\mathbf{k}|\geq K}\left[\langle\frac{a_{\mathbf{k}}}{|\mathbf{k}|}e^{i\mathbf{k}\cdot\mathbf{x}}\rangle+c.c.\right]\\
&\leq\ 4(\frac{4\pi\alpha}{V})^{1/2}\langle\mathbf{p}^2\rangle^{1/2}\sum_{|\mathbf{k}|\geq K}|\mathbf{k}|^{-2}\langle a_{\mathbf{k}}^*a_{\mathbf{k}}\rangle^{1/2}\\
&\leq\ 4(\frac{4\pi\alpha}{V})^{1/2}\langle\mathbf{p}^2\rangle^{1/2}(\sum_{|\mathbf{k}|\geq K}|\mathbf{k}|^{-4})^{1/2}(\sum_{|\mathbf{k}|\geq K}\langle a_{\mathbf{k}}^*a_{\mathbf{k}}\rangle)^{1/2}\\
&=\ 2\varepsilon^{1/2}\langle\mathbf{p}^2\rangle^{1/2}(\sum_{|\mathbf{k}|\geq K}\langle a_{\mathbf{k}}^*a_{\mathbf{k}}\rangle)^{1/2}\\
&\leq\ \varepsilon\langle\mathbf{p}^2\rangle+\sum_{|\mathbf{k}|\geq K}\langle a_{\mathbf{k}}^*a_{\mathbf{k}}\rangle,
\end{aligned}
\tag{10}
$$

again by the Schwarz inequality. (We have taken the limit $V\to\infty$ in the sum.)

The above inequality (10) is an ultraviolet bound. It shows that the Hamiltonian H is bounded below by a new one H_K, i.e., $H\geq H_K$, with

$$
H_K\equiv(1-\frac{8\alpha}{\pi K})\mathbf{p}^2+\sum_{|\mathbf{k}|<K}a_{\mathbf{k}}^*a_{\mathbf{k}}+(\frac{4\pi\alpha}{V})^{1/2}\sum_{|\mathbf{k}|<K}\left[\frac{a_{\mathbf{k}}}{|\mathbf{k}|}e^{i\mathbf{k}\cdot\mathbf{x}}+h.c.\right]. \tag{11}
$$

By completing the square, we have that

$$
a_{\mathbf{k}}^*a_{\mathbf{k}}+(\frac{4\pi\alpha}{V})^{1/2}\left[\frac{a_{\mathbf{k}}}{|\mathbf{k}|}e^{i\mathbf{k}\cdot\mathbf{x}}+h.c.\right]\geq-\frac{4\pi\alpha}{|\mathbf{k}|^2V}, \tag{12}
$$

and if K is chosen so that the coefficient of $\mathbf{p}^2$ vanishes in H_K, i.e., $K=8\alpha/\pi$, then

$$
H\geq H_K\geq-\frac{4\pi\alpha}{V}\sum_{|\mathbf{k}|<K}|\mathbf{k}|^{-2}=-\frac{16}{\pi^2}\alpha^2, \tag{13}
$$

showing that H is indeed bounded below by $O(\alpha^2)$. But to obtain the sharp lower bound, we will take a much larger K, namely $K=(8/\pi c_1)\alpha^{6/5}$. Here and below, the c_i's are constants independent of α.

II. The next step is to localize the electron. Although a-priori the electron is in the box of volume V, it actually can be confined to a box of much smaller size, with only a slight relative increase in its energy. More precisely, we have the following: Let Ψ be any normalized state of the electron and phonons and define $E\equiv\langle\Psi|H_K|\Psi\rangle$. Then, given $\Delta E>0$, there exists a function ϕ of the electron coordinate $\mathbf{x}$ alone (but depending on Ψ), with support in some cube of side length $L=\pi(3/\Delta E)^{1/2}$ such that

$$
\langle\phi\Psi|H_K|\phi\Psi\rangle\Big/\langle\phi\Psi|\phi\Psi\rangle\leq E+\Delta E. \tag{14}
$$

To see this, let $\phi(\mathbf{x})=\prod_{j=1}^3\cos((\Delta E/3)^{1/2}x_j)$ inside the cube of side length $\pi(3/\Delta E)^{1/2}$ centered at the origin and $\phi=0$ outside the cube. Let $\phi_{\mathbf{y}}(\mathbf{x})=\phi(\mathbf{x}-\mathbf{y})$ and consider the integral

$$\int \Big(\langle \phi_{\mathbf{y}} \Psi | H_K | \phi_{\mathbf{y}} \Psi \rangle - (E + \Delta E) \langle \phi_{\mathbf{y}} \Psi | \phi_{\mathbf{y}} \Psi \rangle \Big) d^3 y$$
$$= \int (|\nabla \phi|^2 - \Delta E |\phi|^2)\, d^3 y = 0. \tag{15}$$

(Note here that the cross terms $\nabla \phi_{\mathbf{y}} \nabla \Psi$ vanish after the y-integration.) Evidently, there must be a point $\mathbf{y}$ such that at this point, the integrand on the left side of (15) is non-positive (and where $\langle \phi_{\mathbf{y}} \Psi | \phi_{\mathbf{y}} \Psi \rangle$ is non-zero). This $\phi_{\mathbf{y}}$ is the ϕ that we need. The electron localization is now complete.

For our purposes, we take $\Delta E = c_2 \alpha^{9/5}$, and the assertion above together with the ultraviolet bound then implies that the ground state energy E_0 of H satisfies

$$E_0 \geq \inf_{\Psi}{}' \langle \Psi | H_K | \Psi \rangle - c_2 \alpha^{9/5}, \tag{16}$$

where the infimum is taken over all normalized Ψ's but having their $\mathbf{x}$-support in a cube of side length no larger than $L = (3/c_2)^{1/2} \pi \alpha^{-9/10}$ somewhere in the large volume V.

III. The next step is to group the phonon modes together into blocks, which we take to be cubes with sides of length $P = c_3 \alpha^{3/5}$ or, more precisely, the portion of those cubes lying in the big ball $\{\mathbf{k} : |\mathbf{k}| < K\}$. Let B be a block (cube) of momenta with sides of length $P = c_3 \alpha^{3/5}$ and let $\mathbf{k}_B$ be *any fixed point* within this block whose precise position will be determined later. It is clear that the set of momenta $\{\mathbf{k} : |\mathbf{k}| < K\}$ can be covered by $N \equiv \frac{4}{3} \pi K^3 / P^3 + \textit{lower order} = (2^{11}/(3\pi^2 c_1^3 c_3^3)) \alpha^{9/5} + \textit{lower order}$ such blocks.

Assume that $\mathbf{x}$ itself varies over a cube of side length no bigger than L with center at a point $\mathbf{x}_0$ which we take to be the origin $\mathbf{0}$. (If $\mathbf{x}_0$ is not the origin, phase factors $\exp(\pm i(\mathbf{k} - \mathbf{k}_B) \cdot \mathbf{x}_0)$ standing before $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^*$ in the Hamiltonian H_K are readily eliminated by a unitary transformation involving the phonon variables only.) We have that for $\mathbf{k} \in B$,

$$|e^{i\mathbf{k}\cdot\mathbf{x}} - e^{i\mathbf{k}_B \cdot \mathbf{x}}| \leq |(\mathbf{k} - \mathbf{k}_B) \cdot \mathbf{x}| \leq \frac{3\pi c_3}{2} \Big(\frac{3}{c_2}\Big)^{1/2} \alpha^{-3/10}. \tag{17}$$

Then, for any $\delta > 0$, we have the following inequality, which is obtained by completing the square, as in (12),

$$\sum_B \sum_{\mathbf{k} \in B} \left[\delta a_{\mathbf{k}}^* a_{\mathbf{k}} + \Big(\frac{4\pi\alpha}{V}\Big)^{1/2} \Big[\frac{a_{\mathbf{k}}}{|\mathbf{k}|} (e^{i\mathbf{k}\cdot\mathbf{x}} - e^{i\mathbf{k}_B \cdot \mathbf{x}}) + h.c. \Big] \right]$$
$$\geq -\frac{4\pi\alpha}{\delta V} \left(\frac{3\pi c_3}{2} \Big(\frac{3}{c_2}\Big)^{1/2} \alpha^{-3/10} \right)^2 \sum_{|\mathbf{k}| < K} |\mathbf{k}|^{-2} \tag{18}$$
$$= -\frac{108 c_3^2}{c_1 c_2 \delta} \alpha^{8/5}.$$

We make the choice $\delta = c_4 \alpha^{-1/5}$.

The above inequality (19) permits us to bound H_K (still restricted to states with $\mathbf{x}$-support in a cube of sides with size L) from below in the following way:

$$H_K \geq (1-c_1\alpha^{-1/5})\mathbf{p}^2 + \sum_B \sum_{\mathbf{k}\in B}\Big[(1-c_4\alpha^{-1/5})a_{\mathbf{k}}^* a_{\mathbf{k}} + (\frac{4\pi\alpha}{V})^{1/2}(\frac{a_{\mathbf{k}}}{|\mathbf{k}|}e^{i\mathbf{k}_B\cdot\mathbf{x}} + h.c.)\Big] - \frac{108c_3^2}{c_1c_2c_4}\alpha^{9/5}. \tag{19}$$

Note that, within a single block, the exponential factors multiplying the $a_{\mathbf{k}}$- and $a_{\mathbf{k}}^*$-terms are now *independent* of $\mathbf{k}$. With this in mind, we define, for each block B, a block annihilation operator

$$A_B \equiv (\sum_{\mathbf{k}\in B}|\mathbf{k}|^{-2})^{-1/2}\sum_{\mathbf{k}\in B}\frac{a_{\mathbf{k}}}{|\mathbf{k}|} \tag{20}$$

and its corresponding adjoint A_B^*. These operators are properly normalized boson modes, i.e.,

$$[A_B, A_{B'}^*] = \delta_{B,B'}. \tag{21}$$

Then

$$\sum_{\mathbf{k}\in B} a_{\mathbf{k}}^* a_{\mathbf{k}} \geq A_B^* A_B, \tag{22}$$

and so the operator terms on the right hand side of (19) exceed the operator $H_K^{block} \equiv H_K^{block}(\{\mathbf{k}_B\})$ defined by

$$H_K^{block} \equiv (1-c_1\alpha^{-1/5})\mathbf{p}^2 + \sum_B\Big[(1-c_4\alpha^{-1/5})A_B^*A_B + (\frac{4\pi\alpha}{V}\sum_{\mathbf{k}\in B}|\mathbf{k}|^{-2})^{1/2}(A_B e^{i\mathbf{k}_B\cdot\mathbf{x}} + h.c.)\Big]. \tag{23}$$

Referring to (16) and (19), we can summarize the situation: The ground state energy E_0 of H satisfies

$$E_0 \geq \inf_{\Psi}\sup_{\{\mathbf{k}_B\}}\langle\Psi|H_K^{block}|\Psi\rangle - (c_2 + \frac{108c_3^2}{c_1c_2c_4})\alpha^{9/5}, \tag{24}$$

where the infimum can now even be taken over Ψ's with no restriction on their $\mathbf{x}$-support, and with the $\mathbf{k}_B$'s chosen optimally, depending on Ψ.

IV. In order to get a lower bound on H_K^{block}, we use the technology of coherent states. Let $|\xi\rangle = \pi^{-1/2}\exp(-\frac{1}{2}|\xi|^2 + \xi A^*)|0\rangle$ denote a normalized coherent state for a single harmonic oscillator. In terms of these states one has the identity

$$\exp(\mu A)\exp(\nu A^*) = \int \exp(\mu\xi + \nu\xi^*)|\xi\rangle\langle\xi|d\xi d\xi^*, \tag{25}$$

from which the identities for the operators A and A^*A mentioned in the introduction are readily obtained.

Let Ψ be any normalized state and let $|\xi\rangle = \prod_B |\xi_B\rangle$ denote a tensor product of coherent states of the block modes corresponding to the operators $\{A_B\}$. Set $\Psi_\xi(\mathbf{x}) = \langle\xi|\Psi\rangle_{phonon}$, where the inner product, $\langle\ |\ \rangle_{phonon}$, is just over the phonon variables, not $\mathbf{x}$. Then

$$\langle\Psi|H_K^{block}|\Psi\rangle = \int \langle\Psi_\xi|h_\xi|\Psi_\xi\rangle_{electron} \prod_B d\xi_B d\xi_B^*, \tag{26}$$

where the inner product in the integrand, $\langle\ |\ \rangle_{electron}$, is over the electronic coordinates $\mathbf{x}$, and h_ξ is the Schrödinger operator

$$\begin{aligned} h_\xi \ &\equiv\ (1-c_1\alpha^{-1/5})\mathbf{p}^2 \qquad (27)\\ &+\ \sum_B \Big[(1-c_4\alpha^{-1/5})(|\xi_B|^2-1) + \Big(\frac{4\pi\alpha}{V}\sum_{\mathbf{k}\in B}|\mathbf{k}|^{-2}\Big)^{1/2}(\xi_B e^{i\mathbf{k}_B\cdot\mathbf{x}} + c.c.)\Big]. \end{aligned}$$

Now the supremum over $\mathbf{k}_B$ of (26) exceeds what is obtained by completing the square, namely,

$$\begin{aligned} &\sup_{\{\mathbf{k}_B\}} \int \Big[(1-c_1\alpha^{-1/5})\langle\Psi_\xi|\mathbf{p}^2|\Psi_\xi\rangle_{electron}\\ &\quad -\frac{4\pi\alpha}{(1-c_4\alpha^{-1/5})V}\sum_B\sum_{\mathbf{k}\in B}\frac{|\hat\rho_\xi(\mathbf{k}_B)|^2}{|\mathbf{k}|^2\hat\rho_\xi(\mathbf{0})}\Big]\prod_B d\xi_B d\xi_B^* \ -N, \end{aligned} \tag{28}$$

where $\hat\rho_\xi(\mathbf{k}) = \langle\Psi_\xi|\exp(i\mathbf{k}\cdot\mathbf{x})|\Psi_\xi\rangle_{electron}$ is the Fourier transform of $|\Psi_\xi|^2(\mathbf{x})$. (Here, we can remove the $|\mathbf{k}|<K$ restriction on the $\mathbf{k}$-sum.) We emphasize again that were it not for the grouping of the phonons into blocks, then this coherent state estimate would contain a negative constant equal to the number of phonon modes with $|\mathbf{k}|<K$, which is infinite in the $V\to\infty$ limit, instead of $N = O(\alpha^{9/5})$.

At this point we choose $\mathbf{k}_B$ to be a point in B where the function of $\mathbf{k}$ given by

$$\int \frac{|\hat\rho_\xi(\mathbf{k})|^2}{\hat\rho_\xi(\mathbf{0})}\prod_B d\xi_B d\xi_B^*, \tag{29}$$

is minimal. This point depends on Ψ. With this choice, (28) is, in turn, larger than

$$\begin{aligned} &\int \Big[(1-c_1\alpha^{-1/5})\langle\Psi_\xi|\mathbf{p}^2|\Psi_\xi\rangle_{electron} \qquad (30)\\ &\quad -\frac{4\pi\alpha}{(1-c_4\alpha^{-1/5})V}\sum_{\mathbf{k}}\frac{|\hat\rho_\xi(\mathbf{k})|^2}{|\mathbf{k}|^2\hat\rho_\xi(\mathbf{0})}\Big]\prod_B d\xi_B d\xi_B^* - N. \end{aligned}$$

But the integrand of this integral is $\langle\Psi_\xi|\Psi_\xi\rangle_{electron}\times\mathcal{E}(\Psi_\xi/(\langle\Psi_\xi|\Psi_\xi\rangle_{electron}^{1/2}))$, where $\mathcal{E}(\cdot)$ is just the Pekar functional (2), (but with coefficients altered by $O(\alpha^{-1/5})$); the $\mathbf{k}$-sum is the Fourier series for the Coulomb self-energy term of $\mathcal{E}$. Thus, the integral (30) exceeds $(1-c_1\alpha^{-1/5})^{-1}(1-c_4\alpha^{-1/5})^{-2}E_P(\alpha)$, with $E_P(\alpha)$ being the Pekar minimum energy of (2).

Taking into account the altered coefficients in the Pekar functional, the lower bound (24), and the definition of N, we obtain

$$E_0(\alpha) \geq E_P(\alpha) - \Big(c_2 + \frac{108c_3^2}{c_1c_2c_4} + \frac{2^{11}}{3\pi^2c_1^3c_3^3} + c_5\Big)\alpha^{9/5} - o(\alpha^{9/5}), \tag{31}$$

where $E_P(\alpha) = -c_P\alpha^2$, $c_P = 0.109$, [11], and where $c_5 = (c_1+2c_4)c_P$ accounts for the altered coefficients in the variational principle. This completes the proof of the lower bound. Optimizing the coefficients, we find that the $\alpha^{9/5}$-error term in (31) is no greater than $3.822\alpha^{9/5}$.

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Erratum

Exact Ground State Energy of the Strong-Coupling Polaron*

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We are grateful to Professor Andrey V. Soldatov of the Moscow Steklov Mathematical Institute for calling our attention to an error in our paper. The commutator inequality (8) in our step **I**, namely $|k_j||\langle a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\rangle| \leq 2\langle p_j^2\rangle^{1/2}\langle a_{\mathbf{k}}^* a_{\mathbf{k}}\rangle^{1/2}$, is not correct. Rather, the right side of this inequality should be $\langle p_j^2\rangle^{1/2}(\langle a_{\mathbf{k}}^* a_{\mathbf{k}}\rangle^{1/2} + \langle a_{\mathbf{k}} a_{\mathbf{k}}^*\rangle^{1/2})$ or a related expression. The extra factor $\langle a_{\mathbf{k}} a_{\mathbf{k}}^*\rangle^{1/2}$ with the $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^*$ not in normal order generates uncontrolled mischief with, for example, the right side of the ultraviolet bound (10) containing an additional term $\sum_{|\mathbf{k}|\geq K} 1/2 = \infty$.

The situation is remedied with the help of the method introduced by Lieb and Yamazaki (ref. [14], in our previous paper) to obtain the previous rigorous lower bound on the polaron energy. Our main result, (31), is still valid. Indeed, it is improved slightly.

Define the (vector) operator $\mathbf{Z} = (Z_1, Z_2, Z_3)$ with components

$$Z_j = (\frac{4\pi\alpha}{V})^{1/2} \sum_{|\mathbf{k}|\geq K} k_j \frac{a_{\mathbf{k}}}{|\mathbf{k}|^3} e^{i\mathbf{k}\cdot\mathbf{x}}, \qquad j = 1,2,3. \tag{1}$$

Then the commutator estimate (8) is replaced by

$$\begin{aligned} -(\frac{4\pi\alpha}{V})^{1/2} \sum_{|\mathbf{k}|\geq K} \left[\langle \frac{a_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}}\rangle + c.c.\right] &\equiv -\sum_j \langle [p_j, Z_j - Z_j^*]\rangle \\ \leq 2\langle \mathbf{p}^2\rangle^{1/2}\langle -(\mathbf{Z}-\mathbf{Z}^*)^2\rangle^{1/2} &\leq 2\langle \mathbf{p}^2\rangle^{1/2}\langle 2(\mathbf{Z}^*\mathbf{Z} + \mathbf{Z}\mathbf{Z}^*)\rangle^{1/2} \\ &\leq \varepsilon\langle \mathbf{p}^2\rangle + \frac{2}{\varepsilon}\langle \mathbf{Z}^*\mathbf{Z} + \mathbf{Z}\mathbf{Z}^*\rangle. \end{aligned} \tag{2}$$

Now, each component Z_j can be thought of as a single (unnormalized) oscillator mode having commutator with its adjoint, $[Z_j, Z_j^*] = (4\pi\alpha/V)\sum_{|\mathbf{k}|\geq K} k_j^2 |\mathbf{k}|^{-6} \to 2\alpha/3\pi K$;

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moreover, Z_i and Z_j^* commute for $i \neq j$ (i.e., these modes are orthogonal). Using these facts, we have that

$$\frac{2}{\varepsilon}\langle \mathbf{Z}^*\mathbf{Z} + \mathbf{Z}\mathbf{Z}^* \rangle = \frac{4}{\varepsilon}\langle \mathbf{Z}^*\mathbf{Z} \rangle + \frac{2}{\varepsilon}\left(\frac{2\alpha}{\pi K}\right)$$
$$\leq \sum_{|\mathbf{k}|\geq K} \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle + 3/2 \tag{3}$$

if we choose $\varepsilon = 8\alpha/3\pi K$, which is smaller and better by a factor $1/3$ from the ε in the article. Here we have employed an orthogonal rotation of coordinates bringing $\sum_{|\mathbf{k}|\geq K} a_{\mathbf{k}}^* a_{\mathbf{k}}$ into a form $(4/\varepsilon)\mathbf{Z}^*\mathbf{Z}$+non-negative operators. (Compare Eqs.(21,22) of the article.) Combining these inequalities, we obtain

$$-\left(\frac{4\pi\alpha}{V}\right)^{1/2} \sum_{|\mathbf{k}|\geq K} \left[\langle \frac{a_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} \rangle + c.c.\right] \leq \varepsilon\langle \mathbf{p}^2 \rangle + \sum_{|\mathbf{k}|\geq K} \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle + 3/2. \tag{4}$$

This last inequality is our replacement for the ultraviolet bound (10). It follows that $H \geq H_K - 3/2$, where H_K is as in Eq.(11), but with the coefficient of $\mathbf{p}^2$ given by $(1 - 8\alpha/3\pi K)$ rather than $(1 - 8\alpha/\pi K)$. With the choice $K = 8\alpha/3\pi$, inequality (13) becomes $H \geq -(16\alpha^2/3\pi^2) - 3/2$, a bound at least consistent with a known *upper* bound for the ground state energy linear in α.

The remainder of the article is an analysis of H_K and needs only minor modification. The coefficient of $\mathbf{p}^2$ in Eqs.(19,23,27,28,30) should be $(1 - c_1\alpha^{-1/5}/3)$ and, at the end of the article, $c_5 = (c_1/3 + 2c_4)c_P$. Due to the smaller value of ε defined above, our estimate on the coefficient of $\alpha^{9/5}$ in (31) is slightly improved to 2.337, rather than 3.822 as reported. Of course, our lower bound for the ground state energy is decreased merely by the constant $-3/2$, which is unimportant on a scale of $\alpha^{9/5}$.

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Part VIII

Interacting Bosons

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Simplified Approach to the Ground-State Energy of an Imperfect Bose Gas

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The well-known first two terms in the asymptotic density series for the ground-state energy of a Bose gas, $E_0=2\pi N\rho a[1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}]$, where a is the scattering length of the pair potential, is ordinarily obtained by summing an infinite set of graphs in perturbation theory. We show here how this same series may be obtained by elementary methods. Our method offers the advantages of simplicity and directness. Another advantage is that the hard-core case can be handled on the same basis as a finite potential, no pseudopotential being required. In fact, the analysis of the hard-core potential turns out to be simpler than for a finite potential, as is the case in elementary quantum mechanics. In an Appendix we discuss the high-density situation and show that for a certain class of potentials Bogoliubov's theory is correct in this limit. Thus, Bogoliubov's theory, which is never correct at low density unless a pseudopotential is introduced, is really a high-density theory.

INTRODUCTION

IMPORTANT and often brilliant theoretical investigations by many workers in the past few years have given us considerable insight into the nature of the ground state and low-lying excited states of a many-particle Bose gas at low density with repulsive pairwise forces. While the intermediate density problem is still unsolved, we at least know now how to begin a consistent expansion (possibly divergent) in the density. In appropriate units[1] we have the following well-known formulas for the ground-state energy, E_0, and the energies of the elementary excitations of long wavelength, $\epsilon(\mathbf{k})$:

$$E_0=2\pi N\rho a\{1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}+\cdots\}, \quad (1.1)$$

$$\epsilon(\mathbf{k})=2(\pi\rho a)^{1/2}k+\cdots, \quad (1.2)$$

where N is the number of particles, $\rho=N/V$ is the density, and $a>0$ is the scattering length of the two-body potential. The omitted higher terms in Eq. (1.1) depend upon the shape of the potential as well as the scattering length; Eq. (1.2) is justified if $k\ll(\rho a)^{1/2}$.

While Eqs. (1.1) and (1.2) may now be regarded as well established and, therefore, elementary, it was not always so. The first attempt to find E_0 was based on perturbation theory. Aside from the fact that perturbation theory cannot be justified in this case (E_0 is enormously greater than the spacing between the unperturbed ground and first excited states), it is easily seen that all terms in the perturbation series beyond the second are divergent for any potential. By this is meant that although the terms are not actually infinite, they are proportional to a higher power of N than the first.

Nevertheless, it was held for a long time that the first term in the perturbation series, viz.,

$$E_0'=2\pi N\rho a', \quad (1.3a)$$

where

$$a'=\frac{1}{4\pi}\int v(\mathbf{x})d^3x, \quad (1.3b)$$

was exact,[2] $v(\mathbf{x})$ being the two-body potential. Equation

[1] $\hbar=1$, $m=1$.

[2] We must be careful to define the meaning of exact and approximate as used in this paper. We are interested in calculating E_0 as a function of density for a given fixed potential; we are, therefore, concerned with an asymptotic series in the density whose coefficients, and, indeed, whose entire form are functionals of the potential. As such, Eq. (1.1) is exact in that it gives correctly the first two terms in an asymptotic series. Equations (1.3) and (1.6) are only approximations to that series. If, on the other hand, we regard the potential as being proportional to some parameter, λ, and if we were interested in a double expansion in ρ *and* λ, then Eqs. (1.3) and (1.6) would be exact. We are not interested in this latter type of series because for a large potential, such as a hard core, it is relatively useless. Indeed, there is no need for such a double series, because it is the burden of this paper, as well as of a good deal of previous work, that it is just as easy to generate the former type of single series as the latter double series.

(1.3) was justified on the grounds that E_0' is the expectation value of the Hamiltonian in the unperturbed ground state and that

$$\lim_{\rho\to 0}\langle\psi_0|\psi\rangle=1, \tag{1.4}$$

where ψ_0 and ψ are, respectively, the normalized unperturbed and exact ground-state functions. Equation (1.4), while seemingly reasonable, is only an approximation. The truth is that the left-hand side of Eq. (1.4) is asymptotically zero for large N, not unity.[3–5] It is quite true that ψ approaches unity (i.e., ψ_0) when *all* particles are far apart, but when two or more particles are close together ψ differs appreciably from ψ_0 and this difference does not vanish in the limit $\rho\to 0$. But it is precisely the region when two particles are close together that is needed for evaluating the potential energy. It might be remarked in passing that E_0' must be an upper bound for E_0, a fact borne out by the Spruch, Rosenberg inequality[6]:

$$a<\frac{1}{4\pi}\int v(\mathbf{x})d^3x=a' \tag{1.5}$$

for all $v(\mathbf{x})$ that have no bound states.

The incorrectness of Eq. (1.3) notwithstanding, it is a good approximation to E_0 for those potentials that are relatively shallow compared to their width. Of course, E_0' is completely nonsense for a potential with a hard core, and this gave rise to the view that the hard-core potential was particularly difficult, requiring special tricks and methods—a curious conclusion in view of the especial simplicity of the hard-core potential for two particles.

With E_0' as a starting point, the next problem was to do something about the divergent terms in the perturbation series. Various methods were introduced which in one way or another consisted in summing up an infinite subset of the terms in the perturbation series. A typical, and especially neat example of this procedure is Bogoliubov's method[7] which characteristically gives as a solution Eq. (1.1) with the scattering length, a, replaced thoughout by a'.

$$E_0'+E_0''=2\pi N\rho a'\times\{1+(128/15\sqrt{\pi})[\rho(a')^3]^{1/2}+\cdots\}. \tag{1.6}$$

The method is extraordinarily reasonable, but fails in that it relies on Eq. (1.4) which, as we have seen, is incorrect owing to a misinterpretation of the limiting process $\rho\to 0$.

The next step was the realization that a' is itself the first term in the Born series for a, and with this as a clue it was then seen that each term in the partial summation of the perturbation series mentioned above was itself the first term in a heirarchy which, though it could not be explicitly summed, could be recognized as the Born series for a.[8–10]

Thus, by a very complicated twofold summation of infinite sets of graphs, Eq. (1.1) was finally obtained. At this point, mention must be made of the important work of Lee, Huang, and Yang[11] on the hard-sphere Bose gas. For this problem a', of course, does not exist and so one could not arrive at Eq. (1.6) as a first approximation to Eq. (1.1). But by using the pseudopotential (or alternatively the exact formulation in momentum space given by the author[12]) and then Bogoliubov's method, these authors were able to arrive at Eq. (1.1). At first sight it seems very surprising that Bogoliubov's method, which is never correct and indeed gets worse the deeper the potential, should give the correct answer in the case of an infinite repulsive core. The reason is that by using the pseudopotential as a starting point one has partially solved the problem already, and in fact what has been done is to reverse the order of summing the twofold infinite series mentioned above. An important point to note is that only after Lee, Huang, and Yang had successfully come to grips with the infinite repulsive core, and thereby clearly demonstrated that the scattering length and not a' is the relevant parameter, was progress made in going from Eq. (1.6) to Eq. (1.1) for the finite potential case.

Having said all this by way of a brief historical survey, we may in retrospect consider the following points:

(i) The calculation leading to Eq. (1.1) can by no means be regarded as elementary, although the physical interpretation of the first term, at least, $2\pi N\rho a$, is obvious. It is simply the number of pairs of particles, $\frac{1}{2}N(N-1)$, times the ground energy of two particles, in a box of volume V. Yet to obtain this term one is obliged to sum an infinite series of graphs. There can be no doubt that some plain physics has been obscured by an overwhelming amount of difficult, albeit sophisticated, mathematics. The second term in Eq. (1.1), does not seem to have any very simple physical interpretation, and whatever meaning it does have is obscured by a twofold summation of an infinite series.

(ii) The mathematics itself is certainly not free from internal criticism. For one thing it was thought that one had isolated all the leading order terms when Eq. (1.6) was obtained; this did not prove to be the case. Can we be sure that we have now found all the appropriate terms in arriving at Eq. (1.1)? Secondly, for every term in the series leading to Eq. (1.1), it is easy to see that one has rejected an infinite number of terms each more

[3] L. Van Hove, Physica **18**, 145 (1952).
[4] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[5] N. M. Hugenholtz, Physica, **23**, 481 (1957).
[6] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959).
[7] *The Many Body Problem*, edited by C. De Witt (John Wiley & Sons, Inc., New York, 1959), p. 343.
[8] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117 (1957).
[9] J. T. Beliaev, Zh. Eksperim. i Teor. Fiz. **34**, 417 (1958) [translation: Soviet Phys.—JETP **7**, 289 (1958)].
[10] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).
[11] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).
[12] E. H. Lieb, Proc. Natl. Acad. Sci. U. S. **46**, 1000 (1960).

divergent than the one retained. Thirdly, the series leading to the second term of Eq. (1.6) diverges if one takes the correct order of limits $N\to\infty$ and *then* $\rho a^3\to 0$. This is because the series is a power series in $x=aN/L$, $(L^3=V)$, which, for dimensional reasons, must converge to $x^{5/2}$ for large x—clearly an impossibility. This difficulty was overcome by Lee, Huang, and Yang by a renormalization procedure at high energy; Bogoliubov relied on the fact that the high-momentum components of $v(\mathbf{x})$ went asymptotically to zero. But clearly high-momentum considerations should play no role for particles having very low energy, as in this problem.

(iii) The hard-core problem would seem to be a special case requiring extraordinary care. This is indeed strange in view of the fact that for the many-body problem, as for the elementary two-body problem, the hard-core potential is the only potential for which one can evaluate the potential energy *a priori* and show that it vanishes. All of E_0 is kinetic energy. Indeed one sees at once that the wave function vanishes whenever two or more particles overlap ($|x_i-x_j|\leq a$). Surely this very important piece of information, given *gratis* so to speak, must make the problem simpler rather than more difficult. A more direct and transparent solution of the problem must exist.

We should like to emphasize that we do not mean to be destructively critical or carping, nor to attempt to detract from the importance and usefulness of previous work. But there can be no harm in pointing out failings where they exist and to attempt to do something about them. In any case, if a complicated calculation can be made simpler and brought more into line with elementary notions it can be of benefit for future work. Finally, as in this case where the answer cannot be proved, a simpler derivation increases our confidence in the result.

We shall show how to obtain Eq. (1.1) by a straightforward method involving nothing more complicated than the mathematics of elementary quantum mechanics. [In a subsequent paper we shall discuss Eq. (1.2).] A hint that this is indeed possible is to be found in the fact that after Eq. (1.1) was found, it was shown that the same answer could be obtained variationally by a product trial function[13]

$$\phi=\prod_{\langle i,j\rangle}[1+f(|\mathbf{x}_i-\mathbf{x}_j|)]. \tag{1.7}$$

The method to be given here is not approximate and is not a variational calculation. But we shall show that Eq. (1.1) can be obtained by a consistent and careful use of the superposition approximation familiar in classical statistical mechanics, which in the low-density limit is not an approximation at all but is asymptotically exact.

In an Appendix we shall briefly examine the *high*-density limit and among other things prove that Eq. (1.3) is asymptotically exact for a certain class of finite potentials.

II. SOME GENERAL CONSIDERATIONS

The Hamiltonian of the problem is

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2+\sum_{\langle i,j\rangle}v(|\mathbf{x}_i-\mathbf{x}_j|). \tag{2.1}$$

The first question that arises is what condition must we impose on v in order that the system in its ground state behave like a gas. By this is meant that there must not exist any many-body bound state or, more formally,

$$\lim_{\rho\to 0}E_0=0. \tag{2.2}$$

A necessary and sufficient condition for Eq. (2.2) is not known, but the following is easy to prove:

(i) Necessary conditions are that the scattering length of v be positive and that v does not have a two-body bound state;

(ii) A sufficient condition is that v be everywhere positive.

A necessary and sufficient condition lies somewhere between (i) and (ii) and we shall assume that for the potential in question, Eq. (2.2) is satisfied.

We shall further assume that v is of short range and that a length b exists such that

$$v(\mathbf{r})=0 \quad \text{for} \quad r\geq b. \tag{2.3}$$

Having thus described the problem, we now seek the ground-state energy, E_0, of H as a function of v and the density, in the case of low density. Before proceding to the mathematical analysis it is of central importance to have a clear idea of the relative sizes of the various lengths appearing in the problem.

It is to be assumed, although no one has ever proved this rigorously,[14] that in the limit $N\to\infty$, $V\to\infty$, $N/V=\rho$, E_0 is of the form

$$E_0=N\times\text{function of }\rho. \tag{2.4}$$

Unfortunately, ρ itself is not dimensionless and we must, therefore, look for a characteristic length in the problem. Without attempting to prejudice the issue we shall

[13] See, for example, J. B. Aviles Jr., Ann. Phys. (N.Y.) **5**, 251 (1958) [also, R. Jastrow, Phys. Rev. **98**, 1479 (1955)]. The author treats the hard-sphere problem and was able only to guess at the optimum form of f. This gave a result slightly greater than Eq. (1.1), but it has been subsequently shown [H. A. Bethe (private communication)] that a better choice for f gives exactly Eq. (1.1). K. Hiroike, [Progr. Theoret. Phys. (Kyoto) **27**, 342 (1962)] also derived Eq. (1.1) from a product function by using the hypernetted chain approximation.

[14] There is a heuristic proof of this, however, in O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956). For the hard-sphere case, F. J. Dyson [Phys. Rev. **106**, 20 (1957)] has effectively proved Eq. (2.4) by deriving rigorous upper and lower bounds for E_0 which are of the required form.

Phys. Rev. *130*, 2518–2528 (1963)

choose the scattering length, a, of v (alternatively b could be used). We may, therefore, write

$$E_0=N\rho^{2/3}f(\rho a^3). \tag{2.5}$$

This is not to say that all potentials having the same scattering length give rise to the same energy, although this will indeed prove to be the case at low density. The point is, though, that for a given potential with $a>0$

$$\lim_{x\to 0} f(x)=0, \tag{2.6}$$

a result which follows from examining the variational energy using ψ_0 as a trial function. If we assume that the energy is proportional to the number of pairs of particles at low density then

$$f(x)\sim x^{1/3}, \quad (x \text{ small}), \tag{2.7}$$

a result borne out by the variational calculation.

We may now consider three important lengths appearing in the problem. The first is $l_1=a$ (or b), the second is $l_2=\rho^{-1/3}$ (the average particle spacing), and the third is $l_3=(\rho a)^{-1/2}=l_1^{-1/2}l_2^{3/2}$. As $\rho\to 0$, $l_1/l_2\to 0$ and $l_2/l_3\to 0$.

The significance of l_3 is that it is a kind of correlation length. If Eq. (2.2) is accepted, then

$$E_0=Nk^2\simeq N(l_3)^{-2}, \tag{2.8}$$

where k is the root mean square momentum per particle. Since E_0 is proportional to the number of pairs, k^{-1} or l_3 is thus seen to be of the order of the distance over which two particles are correlated, the distance being much greater than the average particle spacing. Clearly particles tend to decrease their momenta, this distance comes about from a chain of correlations via the intermediate neighbors. Because large distances are associated with low momenta, and because at low densities the particles tend to decrease their momenta, this distance increases with decreasing ρ. Put another way, we see that E_0 is entirely a quantum-mechanical correlation phenomenon; one cannot approximate ψ by a product of single-particle wave packets because either the potential energy would be too great (infinite for hard cores) if the size of a wave packet is larger than l_2 or, in the opposite case, the kinetic energy would be too great ($\sim N\rho^{2/3}$).

The situation here is vastly different from the corresponding Fermi gas at low density. There it is possible to think in terms of wave packets (at least to zeroth order)

$$f(x)=c_1+c_2x^{1/3}, \quad (x \text{ small, Fermi gas}) \tag{2.9}$$

where c_1 and c_2 are constants.

What can we learn from these considerations? The effect we are investigating is caused, so to speak, by a very small length, l_1. But it manifests itself at very large distances. The point is that although the potential is important, its effects at distances of the order of l_1, or even of l_2, is really unimportant. In the sequel, we shall work in configuration space and the analysis will consist in trying to evaluate the asymptotic behavior of certain correlation functions. This asymptotic behavior will then enable us to discover what we need to know about the correlation at distances of the order of l_1 in order to evaluate the energy.

III. CALCULATION OF THE GROUND-STATE ENERGY

We want to find the lowest state of H [see Eq. (2.1)] which is totally symmetric, but this is easily seen to be the absolutely lowest state of H (irrespective of symmetry). The absolutely lowest state of H satisfies

$$\psi\geq 0 \quad \text{for all} \quad \mathbf{x}_1, \cdots, \mathbf{x}_N, \tag{3.1}$$

a fact which can be proved by evaluating the variational energy of $|\psi|$. Equation (3.1) implies the important property

$$\int\cdots\int_V \psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)\prod_{i=1}^{N} d^3x_i\equiv\int\psi>0. \tag{3.2}$$

Since ψ is, therefore, not orthogonal to a totally symmetric function, viz., $f=1$, it must itself be totally symmetric, and, therefore, the contention above is proved. We have tacitly assumed that the ground state is nondegenerate, but this restriction is not necessary.[15,16]

[15] We have glossed over several points of a technical nature which we elucidate here. We do not assume, as other authors have done that the absolute (Boltzmann) ground state of H is nondegenerate. We first prove: (i) among the Boltzmann ground states there is at least one that satisfies $\psi\geq 0$. For a proof, we take the ground-state functions to be real and then take the absolute value of any one of them as a variational trial function. Since this does not change the energy, $|\psi|$ must also be a ground-state function. This device was used by Penrose and Onsager (reference 14) who claim to give the first proof that the Bose ground state is non-negative. This device, however, ignores one difficulty, viz., does $|\psi|$ satisfy the boundary conditions? If the boundary conditions were that $\psi=0$ on the boundary of the box, there would be no problem. But if ψ is periodic, $|\psi|$ will not have a periodic normal derivative if ψ happens to vanish on the boundary. We may overcome this difficulty, however, by the following artifice: If we use strict periodic boundary conditions (cf., reference 17), then we may regard the walls of the box as folded around onto each other (i.e., the square becomes a torus, the cube becomes a hypertorus). In applying the variational principle now, we require only continuity and piecewise differentiability of the wave function, and we do not have to require periodicity of the normal derivative. This latter property will be an automatic consequence of the Euler equations. We can now use $|\psi|$, and the proof of (i) goes through. If ψ is a positive Boltzmann function, then consider $\phi(\mathbf{x})=\sum_P\psi(P\mathbf{x})$, where the summation is on all permutations. ϕ is clearly symmetric and does not vanish identically. In fact, it is non-negative because ψ is. It satisfies the Schrödinger equation and we, therefore, conclude: (ii) among the ground-state Boltzmann functions there is at least one non-negative Bose function. We now wish to prove: (iii) this non-negative Bose functions (call it ϕ) can be taken to have zero momentum. We need this fact in order to establish Eq. (3.6c) above. The proof is as follows: $\phi(\mathbf{x})$ can clearly be periodically extended so that it is defined over all space and satisfies the Schrödinger equation everywhere. By translational invariance of H, if $\phi(\mathbf{x})$ is an eigenfunction, then so is $\phi(\mathbf{x}+\mathbf{a})$ for arbitrary displacement $\mathbf{a}$ of all the particles. Define $h(\mathbf{x})=\int_V\phi(\mathbf{x}+\mathbf{a})d^3a$. The function $h(\mathbf{x})$ does not vanish and is non-negative since $\phi\geq 0$. Also h is a ground-state function and by explicit differentiation it has zero momentum. Q.E.D. We have

Let us integrate both sides of the equation

$$H\psi = E_0\psi. \tag{3.3}$$

It will be seen that for periodic boundary conditions the term $\frac{1}{2}\int(\sum \nabla^2)\psi$ vanishes and, using symmetry, we obtain

$$E_0 = \frac{N(N-1)}{2}\int v(|\mathbf{x}_1-\mathbf{x}_2|)\psi \Big/ \int\psi. \tag{3.4}$$

It will be appreciated that Eq. (3.2) was essential for obtaining Eq. (3.4).

We next define certain correlation or distribution functions which, unlike the customary definitions, are linear in ψ instead of being quadratic. That this is sensible is again a direct consequence of Eq. (3.1)

$$g^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)$$

$$\equiv V^n\int\cdots\int_V \psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)\prod_{j=n+1}^{N} d^3x_j \Big/ \int\psi. \tag{3.5}$$

Periodic boundary conditions[17] imply that g^n is a periodic function of its arguments in V. Recalling the translational invariance of H, we have the following properties for the g^n:

$$g^1(\mathbf{x}_1) = \text{const} = 1, \tag{3.6a}$$

$$g^2 = g^2(\mathbf{x}_1-\mathbf{x}_2), \tag{3.6b}$$

$$g^n(\mathbf{x}_i+\mathbf{a}) = g^n(\mathbf{x}_i), \quad (\mathbf{a}=\text{arbitrary vector}), \tag{3.6c}$$

$$g^n \geq 0 \text{ all } \mathbf{x}_1,\cdots,\mathbf{x}_n, \tag{3.6d}$$

$$\int_V g^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)d^3x_n = Vg^{n-1}(\mathbf{x}_1,\cdots\mathbf{x}_{n-1}). \tag{3.6e}$$

Finally, we need two more obvious facts which, unfortunately, must be assumed. Firstly, since $v(\mathbf{x})$ is a function of $|\mathbf{x}|$—if: (a) n is a fixed integer; (b) $\mathbf{x}_1,\cdots,\mathbf{x}_n$ are confined to a fixed region $R\subset V$; (c) V, and hence N, goes to infinity—then g^n is rotation invariant.

$$g^n(\mathbf{R}\mathbf{x}_i) = g^n(\mathbf{x}_i), \tag{3.6f}$$

where $\mathbf{R}$ is a rotation. In particular[18]

$$g(\mathbf{x}_1-\mathbf{x}_2) = g(|\mathbf{x}_1-\mathbf{x}_2|) = g(r), \quad \text{(large system)}. \tag{3.6g}$$

Equations (3.6f) and (3.6g) would seem to be implied by the principle of independence at large distances [cf. Eq. (3.13) below] but it is difficult to make this connection rigorous. The second property, namely,

$$\lim_{V\to\infty, N/V=\rho} g^n \equiv \bar{g}^n, \text{ exists, } (n \text{ fixed}), \tag{3.6h}$$

means that we can speak of the correlation functions of a finite number of particles in the limit of a large system.[19] This property would appear to follow from Eq. (2.4), but here again a rigorous proof is difficult. Despite (3.6h), however, it will be necessary to some extent to consider the manner in which g^n approaches the limit. We shall return to this point later.

Returning to Eq. (3.4), it may be written

$$E_0 = \tfrac{1}{2}(N-1)\rho\int_V g(\mathbf{x})v(\mathbf{x})d^3x, \tag{3.7}$$

where we have purposely kept $N-1$ instead of N because we are not yet ready to pass to the limit of an infinite system. Equation (3.7) is our rigorous starting point for the calculation of E_0; it is clearly reminiscent of similar formulas in classical statistical mechanics.[20]

At this point we should consider the infinite repulsive core, for in this case Eq. (3.7) is meaningless as it stands. Taking the hard-sphere gas for simplicity, we have

$$-\tfrac{1}{2}\sum\nabla^2\psi = E_0\psi \text{ in } R, \tag{3.8a}$$

$$\psi \equiv 0 \text{ elsewhere and on boundary of } R, \tag{3.8b}$$

where the domain R is defined by

$$R\text{: all } |x_i-x_j| \geq a. \tag{3.9}$$

The wave function and its correlation functions still satisfy Eqs. (3.1), (3.2), (3.5), and (3.6), but now we can integrate Eq. (3.8a) only over R.

$$E_0 = -\tfrac{1}{2}N\int_R \nabla_1^2\psi \Big/ \int_V \psi. \tag{3.10}$$

presented all this detail because the proofs in the literature are incomplete. Dyson (reference 14) quotes Yang to the effect that, since the Boltzmann ground state is non-negative and non-degenerate, all the above properties follow at once. The difficulty is that if the potential is sufficiently pathological there can be degeneracy. For hard spheres in one dimension, the Fermi and Bose ground states are degenerate if N is odd [cf., M. Girardeau, J. Math. Phys. **1**, 516 (1960)]. Indeed, if $\psi=0$ boundary conditions are used, then the ground states of all symmetry classes are degenerate for this problem [cf., E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962)]. Penrose and Onsager claim to prove that the Bose ground state is nondegenerate. This, too, is incorrect if the potential is sufficiently pathological. For a double hard-core potential in one dimension (i.e., $v(x)=\infty$ for $|x|<a$ and $b<|x|<c$, where $a<b<c$, $v(x)=0$ otherwise), for a certain value of L, the length of the box, there will be two degenerate ground-state Bose functions for two particles. Both of these functions may be taken non-negative; they are orthogonal, nevertheless, because when one is nonzero the other vanishes.

[16] Equation (3.2) is not true for the lowest Fermi function and, therefore, the subsequent analysis has to be modified if one wishes to apply it to the Fermi gas. In fact, one does not know *a priori* the spatial symmetry class of the lowest Fermi function, for the total spin need not be zero in the ground state as it is for the free-Fermi gas.

[17] Strict periodicity is implied, meaning that not only is ψ periodic but H as well. Strictly speaking, $v(\mathbf{x})$ must, therefore, be replaced by $\Sigma_{\mathbf{a}}\, v(\mathbf{x}+L\mathbf{a})$ where the summation is over all vectors, $\mathbf{a}$, whose components are integers, and where $V=L\times L\times L$.

[18] Henceforth, we shall use the symbol g in place of g^2.

[19] The same assumption is made in classical-statistical mechanics, and indeed is at the basis of any treatment of large systems.

[20] T. L. Hill, *Statistical Mechanics*, (McGraw-Hill Book Company, Inc., New York, 1956).

Integrating Eq. (3.10) by parts and using Eq. (3.8b) we obtain

$$\Gamma_0=\tfrac{1}{2}N(N-1)\int_V \prod_2^N d^3x_j \times\left\{\int_{r=a} a\mathbf{r}\cdot\nabla_1\psi(\mathbf{x}_2+\mathbf{r},\mathbf{x}_3\cdots\mathbf{x}_N)d\Omega_r\right\}\left(\int_V\psi\right)^{-1}$$

$$=2\pi(N-1)\rho a^2\frac{d}{dr}g(r)\big|_{r=a+} \tag{3.11}$$

upon using (3.6g). Thus,

$$4\pi\int_0^\infty g(r)v(r)r^2dr\to 4\pi a^2\frac{d}{dr}g(r)\big|_{r=a+} \tag{3.12}$$

for hard spheres. We remark in passing that

$$g^n=0 \text{ if any } |\mathbf{x}_i-\mathbf{x}_j|\le a \quad \text{(hard spheres)} \tag{3.6i}$$

by virtue of Eq. (3.8b).

Hence, the hard-sphere case really requires no special treatment. Other integrals similar to Eq. (3.7) will arise and they can all be treated in the same way. We shall, therefore, continue to use these integrals in the hard-sphere case with the understanding that they can (rigorously) be replaced, as in Eq. (3.12), with meaningful expressions.

There is one more property of the correlation functions that needs to be mentioned, viz., the principle of independence at large distances (ILD). Taking g as an example, $\tilde{g}$ satisfies

$$\lim_{|\mathbf{x}|\to\infty}\tilde{g}(\mathbf{x})=\text{const}, \tag{3.13}$$

a fact which, while it cannot be proved,[21] is physically obvious. It means that the correlation between two particles disappears as they move apart. Using Eqs. (3.6a), (3.6b), and (3.6e) the constant in Eq. (3.13) is easily seen to be unity. By the same argument, all $\tilde{g}^n$ satisfy

$$\lim_{|\mathbf{x}_n|\to\infty}\tilde{g}^n(\mathbf{x}_1,\cdots,\mathbf{x}_n)=\tilde{g}^{n-1}(\mathbf{x}_1,\cdots,\mathbf{x}_{n-1}) \tag{3.14}$$

for fixed $\mathbf{x}_1$ through $\mathbf{x}_{n-1}$.

If we, therefore, write

$$\tilde{g}(\mathbf{x})=1-\tilde{u}(\mathbf{x}) \tag{3.15a}$$

and[22]

$$g(\mathbf{x})=\frac{1}{1-\delta}[1-u(\mathbf{x})] =(1+\delta)[1-u(\mathbf{x})]+o(V^{-1}), \tag{3.15b}$$

where

$$\delta=V^{-1}\int_V u(\mathbf{x})d^3x, \tag{3.15c}$$

then

$$\lim_{V\to\infty}u(\mathbf{x})=\tilde{u}(\mathbf{x}), \tag{3.15d}$$

and

$$\lim_{|\mathbf{x}|\to\infty}\tilde{u}(\mathbf{x})=0. \tag{3.15e}$$

The factor $(1-\delta)^{-1}$ in Eq. (3.15b) follows from Eq. (3.6e).

The next step is to find an equation for g. This may be done by operating on g with $-\frac{1}{2}(\nabla_1^2+\nabla_2^2)$ whence, using Eqs (3.3) and (3.5), we obtain[23]

$$[-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)+v_{12}]g(1,2)=E_0g(1,2)-2V^{-1}(N-2) \times\int_V g^3(1,2,3)v_{23}d_3-\tfrac{1}{2}V^{-2}(N-2)(N-3) \times\int\int_V g^4(1,2,3,4)v_{34}d_3d_4\equiv M(1,2). \tag{3.16}$$

Let us consider the order of magnitude of the various terms appearing in Eq. (3.16). If V is very large, we may think of replacing g in the left-hand side by its limit function, which therefore makes the left-hand side of order unity in the volume (note that g^n is dimensionless). Of the three terms on the right-hand side, only the second is of order unity; the other two, being of order V (or N), must cancel each other to order V and leave a residue of order unity. That they indeed cancel may be seen in the following way: In the integrand of the third term we must have $|\mathbf{x}_3-\mathbf{x}_4|<b$, but otherwise the pair (3,4) can be anywhere. Clearly, the major contribution to the integral comes when (3,4) is far from either 1 or 2. In this region we may write $g^4(1,2,3,4)\simeq g(1,2)g(3,4)$ [in analogy with Eq. (3.14)]. Using Eq. (3.7), this contribution, when multiplied by the appropriate factor, yields $-E_0g(1,2)$. The correction, which is thus of order unity, comes from three sources: the presence of the factor $(N-2)(N-3)$ instead of $N(N-1)$; the contribution to the integral when (3,4) is close to either 1 or 2; and the fact that $g^4=\tilde{g}^4+$corrections of $O(V^{-1})$. In this context "close" means $\sim(\rho a)^{-1/2}$, the point being that for a fixed density and a very large system there must be some volume-independent distance beyond which the pairs (1,2) and (3,4) cease to be correlated.

For a large system the function $M(1,2)$ is volume-independent but it is also clear that is essentially proportionally to e, the energy per particle;

$$e=N^{-1}E_0. \tag{3.17}$$

We may, therefore, assume that if we consider ρ to be very small and define

$$G(r)\equiv\lim_{\rho\to0}\tilde{g}(r), \tag{3.18}$$

[21] O. Penrose and L. Onsager, (reference 14) almost succeeded in proving ILD.

[22] $o(x)$ means the quantity in question is of *lower* order than x. $O(x)$ means the same order as x.

[23] In Eq. (3.16) *et seq.* we use the standard notation of statistical mechanics, Cf. reference 20. $g_{12}\equiv g(1,2)\equiv g(\mathbf{x}_1,\mathbf{x}_2)$; $\int d_1\equiv\int d^3x_1$.

then

$$[-\nabla^2+v(\mathbf{x})]G(\mathbf{x})=0. \tag{3.19}$$

This means that in the limit of zero density g is the solution to the zero-energy scattering problem with the potential $v(\mathbf{x})$, a physically satisfying situation. Inserting G into Eq. (3.7) we obtain the result

$$E_0=2\pi N\rho a+o(\rho), \tag{3.20}$$

where a is the scattering length, in agreement with Eq. (1.1). Thus, without further ado, and certainly without summing an infinite set of graphs, we have obtained the leading term in the energy.

For the hard-sphere case we have

$$\begin{aligned} G(r)&=1-a/r, \quad r>a \\ &=0, \qquad r<a. \end{aligned} \tag{3.21}$$

It will be noticed that $G(r)$ has no cutoff length. Physically, the reason is that the cutoff length, $(\rho a)^{-1/2}$, becomes infinite for zero density. Mathematically speaking, the convergence in Eq. (3.18) is nonuniform. To orient ourselves, we may suppose that $\tilde{g}(r)=1-(a/r)\times\exp[-(\rho a)^{1/2}(r-a)]$, a function that has been used in variational calculations.[13] Its limit at zero density is given by Eq. (3.21).

To make further progress, we must attempt to evaluate $M(r)$, and the crucial point here is that we need to know it only for large distances—of the order of $(\rho a)^{-1/2}$. Taking the hard-sphere gas as an example, we have from Eqs. (3.12) and (3.16)

$$e=2\pi\rho a\left(1+\int_a^\infty rM(r)dr\right). \tag{3.22}$$

Thus, if $u(r)$ and hence $rM(r)$ have a certain large cutoff length, l, the major contribution to the integral in Eq. (3.22) will come from distances of the order of l. But at the same time, whatever l may be, it is the distance at which Eq. (3.14) begins to be true.

For the first integral in Eq. (3.16) we see that we need to know $g^3(1,2,3)$ when 2 and 3 are close together and 1 is far removed, by a distance of order l. It seems quite obvious, although we cannot prove it, that in this asymptotic region g^3 may be written

$$g^3(1,2,3)=s[1-w(1,2)][1-w(1,3)][1-w(2.3)], \tag{3.23}$$

where s is a positive constant. If

$$\lim_{V\to\infty} w(\mathbf{x})=\tilde{u}(\mathbf{x}) \quad \text{and} \quad \lim_{V\to\infty} s=1, \tag{3.24}$$

then the assumption, (3.23), is consistent with Eqs. (3.6) and (3.14). But for a finite system we do *not* suppose that $w=u$ for we shall be interested in the difference between w and u which is $o(1)$ in the volume. To determine s and w we use Eq. (3.6e), which is consistent, for although we must integrate x_3 over all space the major contribution to the integral in (3.6e) comes from the asymptotic region where Eq. (3.23) is presumably correct. One easily finds that

$$s=1+3\delta+o(\delta), \tag{3.25}$$

$$w(1,2)=u(1,2)+\frac{1}{V}g(1,2)\int_V u(1,3)u(2,3)d_3+o(\delta). \tag{3.25b}$$

Actually, the V^{-1} corrections to s and w given by Eq. (3.25) will play no role when we evaluate the first integral in Eq. (3.16), for that term is already of order unity in the volume. We obtain (upon passing to the limit of an infinite system)

$$\int_V g^3(1,2,3)v_{23}d_3 \cong g(1,2)\left[\frac{2e}{\rho}-\int_V u(1,3)g(2,3)v_{23}d_3\right], \tag{3.26}$$

where limiting functions and integrals are understood on the right-hand side of Eq. (3.26). We repeat the assertion that Eq. (3.26) is asymptotically correct for large $|\mathbf{x}_1-\mathbf{x}_2|$ and small ρ, and that this is just what is needed in Eq. (3.16) to get the second term in E_0 as a function of ρ.

When we turn to the second integral, however, and apply the same arguments, V^{-1} corrections will be decidedly important. If we write

$$g^4(1,2,3,4)\to t\prod_{(i,j)}[1-h(i,j)] \tag{3.27}$$

and use Eq. (3.6e) twice,[24] we obtain

$$t=1+6\delta+o(\delta), \tag{3.28a}$$

$$h(1,2)=u(1,2)+\frac{2}{V}g(1,2)\int_V u(1,3)u(2,3)d_3+o(\delta). \tag{3.28b}$$

If we now insert Eqs. (3.28) and (3.26) into Eq. (3.16) and combine terms, we get the final equation for g:

$$[-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)+v_{12}]g(1,2)=\rho g(1,2)\{2K(1,2)-\rho L(1,2)\}, \tag{3.29}$$

where

$$K(1,2)=\int_V u(1,3)g(2,3)v_{23}d_3 \tag{3.30a}$$

and

$$L(1,2)=\int\int_V u(1,3)u(2,4)\{g(1,4)g(2,3)-\tfrac{1}{2}u(1,4)u(2,3)\}\times g(3,4)v(3,4)d_3d_4. \tag{3.30b}$$

[24] Unfortunately, if we insert Eq. (3.27) into (3.6e) we will not obtain Eq. (3.23) for, if we did, it would mean that the product *ansatz* would be exact. The best we can do, therefore, is to make g^4 consistent with g.

Furthermore, since Eq. (3.29) is valid only when $|\mathbf{x}_1-\mathbf{x}_2|\gg b$ we can clearly replace the factors $g(2,3)v_{23}$ and $g(3,4)v_{34}$ appearing in Eq. (3.30) by their average value, viz., $\frac{1}{2}e\rho^{-1}$. It might be supposed that we could now replace u and g on the right-hand side of Eq. (3.29) by their zero-density limit [Eq. (3.19)], but this would lead to a divergent integral in Eq. (3.30b). This integral converges, however, because u has a cutoff length. On the other hand, there is no harm in replacing the terms in the parenthesis in Eq. (3.30b) by their zero-density limit. But we can go further than this and replace the entire parenthesis by unity because for the range of $\mathbf{x}_1-\mathbf{x}_2$ in which we are interested, u can be neglected compared to one. This is clear from Eq. (3.21) or (3.19), where we see that up to the cutoff, $u(r)$ is essentially proportional to r^{-1}. In the same spirit, we can replace the factor $g(1,2)$ on the right-hand side of Eq. (3.29) by unity.

Having thus "linearized" Eqs. (3.29) and (3.30), Eq. (3.29) becomes

$$[-\nabla^2+v(r)][1-u(r)]$$
$$=4eu(r)-2e\rho\int_V u(\mathbf{r}-\mathbf{z})u(\mathbf{z})d^3z, \quad (3.31)$$

the last term being clearly a function of $r=|\mathbf{r}|$. It must be emphasized that the linearization of Eq. (3.29) leading to Eq. (3.31) did not alter the long-range part of $M(r)$—at least to leading order in ρ—and that the solution of Eq. (3.31), therefore, will give the next higher term in the energy exactly when it is inserted into Eq. (3.7). But since Eq. (3.31) contains e as a parameter, Eq. (3.7) will become an algebraic equation for e.

Were it not for the presence of $v(r)$, Eq. (3.31) could be solved exactly by a Fourier transformation, because the integral is in the form of a convolution. Nevertheless, since we are only interested in the right-hand side for $r\gg a$, a Fourier transform may still be used to advantage. Taking transforms of both side of Eq. (3.31) we have

$$-k^2u(k)+(2e/\rho)S(k)=4eu(k)-2e\rho u^2(k), \quad (3.32)$$

where

$$u(k)=\int u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}d^3r \quad (3.33a)$$

and

$$S(k)=\frac{\rho}{2e}\int g(\mathbf{r})v(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}d^3r. \quad (3.33b)$$

The solution to Eq. (3.32) is

$$\rho u(k)=(x^2+1)-[x^4+2x^2+1-S(k)]^{1/2}$$
$$\sim\tfrac{1}{2}S(k)[x^{-2}-x^{-4}+O(x^{-6})], \quad \text{large } k, \quad (3.34)$$

where

$$4ex^2=k^2. \quad (3.35)$$

We now write

$$u=u_1+u_2, \quad (3.36)$$

where

$$\rho u_1(k)=(2e/k^2)S(k). \quad (3.37)$$

Since

$$u(r)=\frac{1}{2\pi^2}\int_0^\infty k^2dk\,u(k)\frac{\sin kr}{kr}, \quad (3.38)$$

we see that $u_1(r)$ is the solution to the equation

$$-\nabla^2u_1(\mathbf{x})=g(\mathbf{x})v(\mathbf{x}), \quad (3.39)$$

which means that

$$u_1(r)=(e/2\pi\rho)(1/r), \quad r\geq b, \quad (3.40)$$

by Gauss' theorem and Eq. (3.7).

Now because $S(k)\to 0$, as $k\to\infty$, and since $u_1(k)$ is just the asymptotic part of $u(k)$,we see that $u_2(k)$ vanishes at least like k^{-4} for large k. Furthermore, $S(k=0)=1$, and $S(k)$ will not depart from unity until k is of the order of b^{-1}, at which point $k^2u_2(k)$ is negligible. Therefore, to the order in which we are interested

$$u_2(r)=4\frac{e^{3/2}}{\pi^2\rho}\int_0^\infty dx\,x^2\frac{\sin\lambda xr}{\lambda xr}$$
$$\times\left(x^2+1-x(x^2+2)^{1/2}-\frac{1}{2x^2}\right), \quad (3.41)$$

where $\lambda=2\sqrt{e}$. It will be seen that for r of the order of b or less, $u_2(r)$ is a very slowly varying function and, for the accuracy we need, it may be replaced by its value at $r=0$. Later on we shall discuss the function defined by Eq. (3.41), but for the present, it is an elementary exercise to deduce that

$$u_2(0)=-\frac{32\sqrt{2}}{15\pi^2\rho}e^{3/2}\approx-\frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}, \quad (3.42)$$

the last expression being obtained by replacing e by its leading term [Eq. (3.20)].

The essential point to notice is this: As we see from Eq. (3.19), for small values of r the function g(or u) oscillates, and this oscillation is contained almost entirely in u_1. Since $g=1-u_1-u_2$

$$-\nabla^2g\approx\nabla^2u_1 \quad (3.43)$$

and hence, from Eq. (3.39),

$$-\nabla^2g+vg=0 \quad \text{for} \quad r\lesssim\rho^{-1/3}. \quad (3.44)$$

Equation (3.44) tells us that for small r, g is proportional to G, the first approximation to g, and is, therefore, very sensitive to the details of $v(r)$. But for large r, g is very different, being given by two universal functions, u_1 and u_2, which contain the energy as their only parameter. Thus,

$$g(r)=AG(r) \quad \text{for} \quad r\lesssim\rho^{-1/3}, \quad (3.45a)$$

where A is some constant, and

$$g(r)=A(1-a/r) \quad \text{for} \quad b\leq r\lesssim\rho^{-1/3}, \tag{3.45b}$$

$$=1-u_2(r)-u_1(r)\approx 1-u_2(0)-e/2\pi\rho r. \tag{3.45c}$$

Equating coefficients in Eq. (3.45), we obtain

$$A=1-u_2(0) \tag{3.46a}$$

and

$$e/2\pi\rho a=A. \tag{3.46b}$$

Thus,

$$e=2\pi\rho a\{1+(128/15\sqrt{\pi})(\rho a^3)^{1/2}+o[(\rho a^3)^{1/2}]\}, \tag{3.47}$$

in conformity with Eq. (1.1). We have thus, established that the first correction to e depends only upon the scattering length of v; higher corrections will clearly involve the effective range.[25] It is tempting, however, to solve Eq. (3.46) exactly. That is,

$$e/2\pi\rho a=1-u_2(0)=1+(32\sqrt{2}/15\pi^2\rho)e^{3/2}. \tag{3.48}$$

This is a cubic equation whose positive root has the correct general behavior up to $e=6\pi\rho a$, $\rho a^3=(\pi/3)(5/64)^2$, and then becomes complex. This value of ρa^3 is only about $\frac{1}{2}\%$ of the value at tight packing, viz., $\sqrt{2}$. In order to make any further progress it would be necessary to go back to Eq. (3.29)—clearly a job for machine computation. We can, however, learn something from Eq. (3.48). For the range of density over which it makes sense, it probably gives a better approximation for e than the first two terms in the asymptotic series, (3.47). At the limiting density mentioned above, it gives $e=6\pi\rho a$ while (3.47) gives $e=2\pi\rho a(1+2/3\sqrt{3})$. We may thus conclude that the $e(\rho)$ curve rises much more sharply than (3.47) would indicate, and that (3.47) is probably numerically accurate only for a much smaller density than the above limiting density.

We now return to the evaluation of $u_2(r)$ [Eq. (3.41)], that part of u which depnds only upon the scattering length. We define

$$R=(8e)^{1/2}r\approx 4(\pi\rho a)^{1/2}r \tag{3.49a}$$

and

$$u_2(r)=\frac{8e}{\pi^2\rho r}f(R)\approx\frac{16a}{\pi r}f(R). \tag{3.49a}$$

The integral in Eq. (3.41) may be transformed into a contour integral around the cut $(\sqrt{2}i-\sqrt{2}i)$ with the result that

$$f(R)=\int_0^1 dz\, z^2(1-z^2)^{1/2}(e^{-Rz}-1). \tag{3.50}$$

[25] It is clear how one could get higher corrections to Eq. (1.1) using the formalism presented here. One can derive an equation for g^3 and g^4 in analogy with (3.16) and solve them using superposition. Then insert the results into Eq. (3.16) and solve for a new $g(1,2)$. On the other hand, as Eq. (3.48) *et seq.* shows, such an asymptotic expansion is probably of academic interest only. A much better thing to try to do is to solve the full nonlinear equation, (3.29).

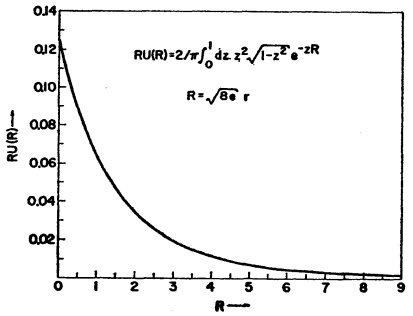

FIG. 1. The universal part of the two-particle correlation function, $g(r)\equiv 1-u(r)$, is given by $u(r)=[4(2e)^{3/2}/\pi\rho]U(R)$ $\approx 32(\pi\rho)^{1/2}a^{3/2}U(R)$. The ground-state energy per particle is $e\approx 2\pi\rho a$, and the dimensionless variable R is given by $R=(8e)^{1/2}r\approx 4(\pi\rho a)^{1/2}r$. This definition of $u(r)$ is valid for $r>b$, where b is the distance beyond which the two-body potential vanishes. $b\ll\rho^{-1/3}\ll(\rho a)^{-1/2}$. For $0<r<b$, $g(r)$ is the zero-energy scattering function of the potential.

It is elementary to deduce that, for small R,

$$f(R)=-(2/15)R+O(R^2), \tag{3.51}$$

which, when combined with Eq. (3.49), gives Eq. (3.42). It is also elementary to integrate the second term in parenthesis in Eq. (3.50). This yields a constant of course which, when combined with Eq. (3.49), gives $-e(2\pi\rho r)^{-1}$. But this is just the value of $-u_1(r)$ for $r\geq b$. Hence, for $r\geq b$

$$u(r)=\frac{8e}{\pi^2\rho r}\int_0^1 dz\, z^2(1-z^2)^{1/2}e^{-Rz} \tag{3.52}$$

$$\equiv(4/\pi\rho)(2e)^{3/2}U(R).$$

Equation (3.52) is not valid for $r<b$—it goes like R^{-1} and this is incorrect. Instead, Eq. (3.44) defines u for $r\leq b$. Equation (3.46) insures that in the overlap region $(b\leq r\lesssim\rho^{-1/3})$, these two definitions of $u(r)$ are substantially the same. Furthermore, the effective cutoff length of $u(r)$ is seen to be of the order of $l_3=(\rho a)^{-1/2}$, in agreement with Sec. II.

The integral in Eq. (3.52) can be evaluated in terms of Bessel functions. The result is:

$$U(R)=R^{-3}\{R[I_1(R)-L_1(R)]$$

$$-3[I_2(R)-L_2(R)]\}, \tag{3.53}$$

where $L(R)$ is the modified Struve function and $I(R)$ is the modified Bessel function of the first kind.[26] Both $I(R)$ and $L(R)$ go to ∞ as $R\to\infty$, but their difference is finite. When R is large, $U(R)\sim R^{-4}$—a result found previously by Lee, Huang, and Yang in the hard-sphere case.[11] The function $U(R)$ is plotted in Fig. 1.

[26] A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 38; *Tables of Integral Transforms*, edited by A. Erdelyi (McGraw-Hill Book Company, Inc., New York, 1954), Vol. I, p. 138, No. 12.

APPENDIX

The High-Density Limit

While Bogoliubov's result, Eq. (1.3), is never correct at low density because it replaces the scattering length, a, by a', the first Born approximation to a, we wish to show here that it is correct in the limit of high density for a certain class of finite potentials. The discussion presented here is independent of the previous results of this paper, but it is interesting in that it shows that Bogoliubov's original point of view, which seems at first sight very reasonable, is really a high-density *ansatz*.

The basic idea behind Bogoliubov's theory is that in some sense the interacting particles behave like free particles to a first approximation. Although at low density $\psi \simeq \psi_0$ when the particles are far apart, as we have seen the important region to consider is when two particles are close together. In this latter region ψ is different from ψ_0 and the difference does not vanish as $\rho \to 0$.

Let us now inquire what happens as the density gets very large. For a potential with a hard core one can only go up to the critical density, $\rho_c a^3 = \sqrt{2}$, at which point the ground-state energy, E_0, becomes infinite. For a finite potential, on the other hand, as we go to high density (such that $\rho b^3 \gg 1$, where b = range of the potential) basically one of two things can happen:

(i) Some definite type of particle configuration (presumably a lattice) may be preferred. In this case, the particles will become localized with respect to each other (i.e., particle correlations will become important) and the kinetic energy will increase with density and become quite large, possibly unbounded. The large kinetic energy will be compensated by the favorable potential energy of the configuration. Such a situation presumably occurs in the hard-core case shortly before reaching the critical density.

(ii) No special configuration is preferred because the advantage of a low potential energy configuration is outweighed by the high kinetic energy required to achieve it. In this case the particles are "smeared" and the kinetic energy goes to zero as $\rho \to \infty$. Owing to the high density, each particle "sees" a constant potential—the average potential of its many neighbors. It is in this case that we may think of the wave function as approximately the noninteracting wave function, ψ_0, because correlations become less important as the density increases. For this case to hold it is not essential that the potential be everywhere repulsive. As we shall see, it can even have a two-body bound state.

We shall show here that there is a class of potentials for which case (ii) holds, and for which Bogoliubov's theory is then valid—at least for the ground-state energy. Let $v(\mathbf{r})$ be the two-body potential, and $\nu(\mathbf{k})$ be its Fourier transform defined by

$$\nu(\mathbf{k}) = \int v(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3r. \tag{A1}$$

The potentials we wish to consider satisfy

$$v(0) = \alpha = \text{finite}, \tag{A2a}$$

$$\nu(\mathbf{k}) \geq 0, \text{ all } \mathbf{k}. \tag{A2b}$$

A repulsive Gaussian potential, for example, is of this class. Notice that we do not assume $v(\mathbf{r}) > 0$, or even that the scattering length is positive. Consider the potential which is a repulsive square well in momentum space:

$$\begin{aligned} \nu(\mathbf{k}) &= \lambda, \quad k < K \\ &= 0, \quad k > K, \end{aligned} \tag{A3a}$$

$$v(\mathbf{r}) = -\lambda(K/2\pi^2 r^2)[\cos rK - (1/rK)\sin rK], \tag{A3b}$$

where λ and K are positive constants. This potential can have a two-body bound state if λ is sufficiently large, yet it is in our class.

We propose to find an upper and lower bound for the ground-state energy. An upper bound is obtained from the variational principle using $\psi_0 = 1$, viz.,

$$e < \tfrac{1}{2}\rho\nu(0), \tag{A4}$$

where $E_0 = Ne$. For the lower bound we use the fact that the kinetic energy is positive definite, whence

$$e > N^{-1} \min_{(\mathbf{x}_1, \cdots, \mathbf{x}_N)} \sum_{(i,j)} v_{ij} \equiv B. \tag{A5}$$

Equation (A5) states that $E_0 >$ minimum potential energy. Let the minimum configuration occur at $\mathbf{x}_i = \mathbf{a}_i$. Then

$$B = \min_{\{\mathbf{a}_i\}} \frac{1}{2N} \int\int \phi^*(\mathbf{x}) v(x-y) \phi(\mathbf{y}) d^3x d^3y - \tfrac{1}{2}\alpha, \tag{A6}$$

where

$$\phi(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{a}_i). \tag{A7}$$

If $\tilde{\phi}(\mathbf{k})$ is the Fourier transform of $\phi(\mathbf{x})$, [cf., Eq. (A1)], then

$$B = (2NV)^{-1} \sum_{\mathbf{k}} |\tilde{\phi}(\mathbf{k})|^2 \nu(\mathbf{k}) - \tfrac{1}{2}\alpha \tag{A8a}$$

$$> \tfrac{1}{2}\rho\nu(0) - \tfrac{1}{2}\alpha, \tag{A8b}$$

where the last inequality follows from (A2b) and the fact that $\tilde{\phi}(0) = N$, whatever $\{\mathbf{a}\}$ may be. Thus, combining (A4) and (A8),

$$\tfrac{1}{2}\rho\nu(0) > e > \tfrac{1}{2}\rho\nu(0) - \tfrac{1}{2}\alpha, \text{ (all } \rho), \tag{A9}$$

Since α = finite, we have proved that the asymptotic form of e is $\frac{1}{2}\rho\nu(0)$. Moreover, with upper/lower bound

formulas for expectation values,[27] it is an easy matter, using the above inequalities, to prove that

$$t<\tfrac{1}{2}\alpha \quad \text{(all } \rho\text{)},$$
$$\tfrac{1}{2}\rho\nu(0)>v>\tfrac{1}{2}\rho\nu(0)-\tfrac{1}{2}\alpha \quad \text{(all } \rho\text{)}, \tag{A10}$$

where t is the kinetic energy and v the potential energy per particle. Equation (A10) establishes that the kinetic energy remains bounded at high density. Actually, using a better upper bound than (A4), we shall show that for large ρ

$$t=o(\rho^{\epsilon}), \tag{A11a}$$
$$v=\tfrac{1}{2}\rho\nu(0)-\tfrac{1}{2}\alpha+o(\rho^{\epsilon}), \tag{A11b}$$
$$e=\tfrac{1}{2}\rho\nu(0)-\tfrac{1}{2}\alpha+o(\rho^{\epsilon}), \tag{A11c}$$

where ϵ=positive constant.

Equation (A11b) is a bit surprising in that we have proved that $\frac{1}{2}\rho\nu(0)-\frac{1}{2}\alpha$ is actually less than the minimum potential energy. The explanation is as follows: From the fact that $t\to 0$, we see that the minimum potential energy is not very different from the potential energy in a perfectly smeared wave function, i.e., $\psi_0=1$. In this case, the potential seen by a test charge would be $\rho\nu(0)$. The potential seen by one of the particles of the gas itself would be $\rho\nu(0)-\alpha$, because α is the effect of a particle on itself. Finally, dividing by two because we have double counted, we obtain the expression (A8b) for B. In other words, as regards the value of B itself, (A8b), in fact, gives correctly the first two terms in an asymptotic series for B in terms of ρ. On the other hand, from the fact that (A8b) was obtained without explicit reference to the minimum potential configuration $\{\mathbf{a}\}$, we see that the potential has an exceedingly broad minimum which in the limit of high density may be taken to be virtually the entire configuration space. This leads in turn to the result that $\lim_{\rho\to\infty} t=0$.

To obtain an improvement on (A4), and thereby establish Eqs. (A11), we turn to the variational calculation of Girardeau.[28] Following the notation of that paper, we see that if we choose $\phi(\mathbf{k})=1$ and set $\rho_0=\rho$ the integrals involving $\nu(\mathbf{k})$ would give us exactly $-\frac{1}{2}\alpha$. We cannot do this, however, for two reasons: The integrals involving k^2, I_1, and I_2, all of which are positive, would diverge; and $\rho-\rho_0$ would also diverge. But by choosing $\phi(\mathbf{k})=1-\rho^{-\alpha}f(k)$, for a suitable choice of α and $f(k)$ we can obtain an upper bound for e of the form of the right-hand side of Eq. (A11c). We omit the details here. Combining the result with (A9) we thus prove Eqs. (A11).

We turn now to the predictions of Bogoliubov's theory.[7] One has $e=e'+e''$, where

$$e'=\tfrac{1}{2}\rho\nu(0), \tag{A12a}$$

$$e''=(16\pi^3\rho)^{-1}\int d^3k \times\{\tfrac{1}{2}k[k^2+4\rho\nu(\mathbf{k})]^{1/2}-\tfrac{1}{2}k^2-\rho\nu(\mathbf{k})\}. \tag{A12b}$$

In the low-density limit we obtain Eq. (1.6) for any potential such that $\nu(\mathbf{k})/k^2$ is integrable. Lee, Huang, and Yang[11] were the first to obtain the famous factor $128/15\sqrt{\pi}$, but this factor is already implicit in Eq. (A12) which antedates their work.

For high density, the major contribution to e'' comes from the last term in the integrand and the total result is in agreement with (A11c). It is to be noted that both in Eq. (A11c) and in Eq. (A12b) the correction of $o(\rho^{\epsilon})$ is positive.

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Bose-Einstein quantum phase transition in an optical lattice model

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Bose-Einstein condensation (BEC) in cold gases can be turned on and off by an external potential, such as that presented by an optical lattice. We present a model of this phenomenon which we are able to analyze rigorously. The system is a hard core lattice gas at half of the maximum density and the optical lattice is modeled by a periodic potential of strength λ. For small λ and temperature, BEC is proved to occur, while at large λ or temperature there is no BEC. At large λ the low-temperature states are in a Mott insulator phase with a characteristic gap that is absent in the BEC phase. The interparticle interaction is essential for this transition, which occurs even in the ground state. Surprisingly, the condensation is always into the $\mathbf{p}=\mathbf{0}$ mode in this model, although the density itself has the periodicity of the imposed potential.

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I. INTRODUCTION

One of the most remarkable recent developments in the study of ultracold Bose gases is the observation of a reversible transition from a Bose-Einstein condensate to a state composed of localized atoms as the strength of a periodic, optical trapping potential is varied [1,2]. This is an example of a quantum phase transition [3] where quantum fluctuations and correlations rather than energy-entropy competition is the driving force and its theoretical understanding is quite challenging. The model usually considered for describing this phenomenon is the Bose-Hubbard model and the transition is interpreted as the superfluid-insulator transition that was studied in Ref. [4] with an application to ^{4}He in porous media in mind. The possibility of applying this scheme to gases of alkali-metal atoms in optical traps was realized in Ref. [5]. The paper [6] reviews these developments and many recent papers, e.g., Refs. [7–15] are devoted to this topic. These papers contain also further references to earlier work along these lines.

The investigations of the phase transition in the Bose-Hubbard model are mostly based on variational or numerical methods and the signal of the phase transition is usually taken to be that a variational ansatz with a sharp particle number at each lattice site leads to a lower energy than a delocalized Bogoliubov state. On the other hand, there exists no rigorous proof, so far, that the true ground state of the model has off-diagonal long-range order at one end of the parameter regime that disappears at the other end. In the present paper we study a slightly different model where just this phenomenon can be rigorously proved and which, at the same time, captures the salient features of the experimental situation.

The model is that of a hard core gas on a cubic lattice at half filling (i.e., when the particle number is half the number of sites). The "optical lattice" is modeled simply by a periodic, one-body potential $\lambda(-1)^{\mathbf{x}}$, where $(-1)^{\mathbf{x}}=+1$ on the A sublattice and $(-1)^{\mathbf{x}}=-1$ on the B sublattice. Thus the Hamiltonian, expressed through bosonic creation and annihilation operators, equals

$$H=-\frac{1}{2}\sum_{\langle \mathbf{xy}\rangle}(a_{\mathbf{x}}^{\dagger}a_{\mathbf{y}}+a_{\mathbf{x}}a_{\mathbf{y}}^{\dagger})+\lambda\sum_{\mathbf{x}}(-1)^{\mathbf{x}}a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}+U\sum_{\mathbf{x}}a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}(a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}-1). \quad (1)$$

The sites $\mathbf{x}$ are in a d-dimensional hypercubic lattice, and $\langle \mathbf{xy}\rangle$ stands for pairs of nearest neighbors. The case considered in this paper is the hard-core interaction $U=\infty$. Apart from the periodic potential, this is also the Bose-Hubbard model with infinite on-site repulsion.

Note that in our model the troughs of the optical potential correspond to the B sublattice where the periodic potential is negative, and the crests correspond to the A sublattice. Often in the Bose-Hubbard model the whole lattice itself is used to approximate the troughs alone. Roughly speaking, half filling in our model corresponds to filling factor 1 in the Bose-Hubbard approximation.

Physically, there are two parameters in the problem. One is the strength of the potential generated by the optical lattice (which is denoted by λ in our model); the other is the strength of the interparticle interaction (denoted by U in the Hubbard model). The Bose-Hubbard model addresses a

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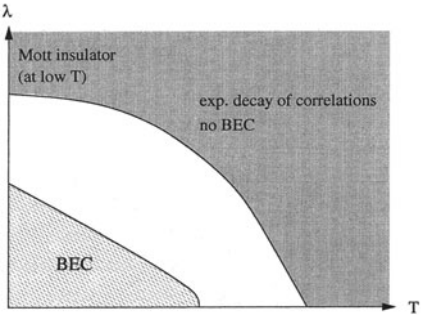

FIG. 1. Schematic phase diagram at half filling.

tight-binding limit in which the particles are located primarily in the troughs of the optical potential. Our model addresses the $U=\infty$ situation. The overall physical properties of the two models ought to be similar.

As is well known, the model (1) with $U=\infty$ can also be viewed as the XY model of a spin-1/2 system [16]. The periodic potential then corresponds to a staggered magnetic field. This will be explained in the next section.

We are able to prove the following facts rigorously for three or more dimensions. The λ-T-phase diagram at half filling (e.g., mean density $\varrho=\frac{1}{2}$) is shown schematically in Fig. 1.

(i) If both λ and the temperature T are small, then there is Bose-Einstein condensation (BEC). In this parameter regime the one-body density matrix has exactly one large eigenvalue (in the thermodynamic limit), and the corresponding condensate wave function is $\varphi(\mathbf{x})=$const.

(ii) If either T or λ is big enough, then the correlation function (the one-body density matrix) decays exponentially, and hence there is *no BEC*. In particular, this applies to the ground state ($T=0$) for λ big enough.

(iii) The Mott insulator phase is characterized by a gap, i.e., a jump in the chemical potential (at zero temperature). We are able to prove this, at half filling, for big enough λ. More precisely, there is a cusp in the dependence of the ground state energy on the number of particles; adding or removing one particle costs a nonzero amount of energy. We also show that there is no such gap whenever there is BEC.

(iv) The interparticle interaction is essential for items (ii) and (iii). Noninteracting bosons *always display BEC* for low, but positive T (which depends on λ, of course).

(v) Whenever there is BEC the off-diagonal long-range order is constant in our model, i.e., $\langle a_{\mathbf{x}}^{\dagger}a_{\mathbf{y}}\rangle \approx$ const for large $|\mathbf{x}-\mathbf{y}|$. (The particle-hole symmetry at half filling is important for this.) On the other hand, for all $T\geq 0$ and all $\lambda>0$ the diagonal part of the one-body density matrix $\langle a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}\rangle$ is not constant. Its value on the A sublattice is constant, but strictly less than its constant value on the B sublattice (for a finite system with periodic boundary conditions) and this discrepancy survives in the thermodynamic limit.

We give explicit expressions for the curves, sketched in Fig. 1, defining the regimes for which the above statements are proved here [see Eqs. (3) and (14) below]. We are not able to make a rigorous statement about the intermediate regime, but we believe that there is only a critical line separating the BEC and the Mott insulator phases.

We focus here on lattice dimensions $d\geq 3$ but, using the technique employed in Ref. [17], an extension to the ground state in two dimensions is possible. Other possible extensions are mentioned in the next section.

II. DETAILED DESCRIPTION OF THE MODEL

We write the Hamiltonian (1) of the lattice gas with $U=\infty$ in terms of the creation and annihilation operators, $a_{\mathbf{x}}^{\dagger}$ and $a_{\mathbf{x}}$, for particles at lattice site $\mathbf{x}\in\Lambda$, with Λ a finite hypercubic lattice with L^d sites, L being an even integer. We impose periodic boundary conditions. Because of the hard-core condition, there is at most one particle at each site, and thus the creation and annihilation operators can be represented as 2×2 matrices with

$$a_{\mathbf{x}}^{\dagger}\leftrightarrow\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad a_{\mathbf{x}}\leftrightarrow\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}\leftrightarrow\begin{pmatrix}1&0\\0&0\end{pmatrix},$$

for each $\mathbf{x}\in\Lambda$. The correspondence with the spin matrices

$$S^1=\frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad S^2=\frac{1}{2}\begin{pmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{pmatrix},\quad S^3=\frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

is

$$a_{\mathbf{x}}^{\dagger}=S_{\mathbf{x}}^1+\mathrm{i}S_{\mathbf{x}}^2\equiv S_{\mathbf{x}}^{+},\quad a_{\mathbf{x}}=S_{\mathbf{x}}^1-\mathrm{i}S_{\mathbf{x}}^2\equiv S_{\mathbf{x}}^{-},$$

and hence $a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}=S_{\mathbf{x}}^3+\frac{1}{2}$. Adding a convenient constant to make the periodic potential positive, the Hamiltonian (1) for $U=\infty$ is thus equivalent to

$$\begin{aligned}H&=-\tfrac{1}{2}\sum_{\langle\mathbf{xy}\rangle}\left(S_{\mathbf{x}}^{+}S_{\mathbf{y}}^{-}+S_{\mathbf{x}}^{-}S_{\mathbf{y}}^{+}\right)+\lambda\sum_{\mathbf{x}}\left[\tfrac{1}{2}+(-1)^{\mathbf{x}}S_{\mathbf{x}}^3\right]\\&=-\sum_{\langle\mathbf{xy}\rangle}\left(S_{\mathbf{x}}^1S_{\mathbf{y}}^1+S_{\mathbf{x}}^2S_{\mathbf{y}}^2\right)+\lambda\sum_{\mathbf{x}}\left[\tfrac{1}{2}+(-1)^{\mathbf{x}}S_{\mathbf{x}}^3\right].\end{aligned}\tag{2}$$

As explained in the Introduction, $(-1)^{\mathbf{x}}=\pm 1$ on alternating sites. Without loss of generality we may assume $\lambda\geq 0$. Note that the subtraction of the "diagonal" terms in the kinetic energy has the effect of a chemical potential and as a consequence the unique ground state of Eq. (2) has particle number $N=\frac{1}{2}|\Lambda|$. We postpone the proof of this assertion to Appendix A.

The presence or absence of Bose-Einstein condensation is expressed through the reduced one-particle density matrix

$$\gamma(\mathbf{x},\mathbf{y})=\langle a_{\mathbf{x}}^{\dagger}a_{\mathbf{y}}\rangle,$$

where $\langle\cdot\rangle$ denotes the expectation value in the *grand canonical* thermal equilibrium state or the ground state considered. BEC occurs (by definition) if the $L^d\times L^d$ matrix $\gamma(\mathbf{x},\mathbf{y})$ has an eigenvalue of order N in the thermodynamic limit $\Lambda\to\infty$, $N\to\infty$, with $\varrho=N/|\Lambda|$ fixed.

We shall prove that for $\varrho=1/2$ and $d\geq 3$ the thermal equilibrium state of (2) shows Bose-Einstein condensation for small λ and low temperature T, while for large λ or T the condensation disappears. For $d=2$ this is true only in the

ground state. Here, ϱ stands for the average density, since we are using the grand-canonical ensemble where the particle number is not fixed. Note that we are not dealing here with a dilute system and the condensation is always depleted, even in the ground state.

We remark that the Hamiltonian (2) is invariant under the following two unitary transformations, which will be used throughout the paper. (i) Uniform rotation around the S^3 axis, in particular the map $S^1_{\mathbf{x}} \to -S^1_{\mathbf{x}}$ and $S^2_{\mathbf{x}} \to -S^2_{\mathbf{x}}$ at all sites. The corresponding conserved generator is the total particle number. (ii) The particle-hole symmetry, which corresponds to: $S^1_{\mathbf{x}} \leftrightarrow S^2_{\mathbf{x}}$, $S^3_{\mathbf{x}} \to -S^3_{\mathbf{x}}$ at all sites, followed by a unit-vector translation in any of the lattice directions. For the latter symmetry the half filling is essential.

Our analysis of the system proceeds via the following steps. In Sec. III we prove infrared bounds on the two-point function $\langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}} \rangle$ in momentum space. The essential ingredient here is *reflection positivity* [18,19] of the Hamiltonian (2) and the closely related property of *Gaussian domination* [18–20]. The bound obtained depends on λ and the temperature. A sum rule fixes the sum over $\mathbf{p}$ of the two-point function and the infrared bound leads to the conclusion that for small λ and low temperatures the contribution from $\mathbf{p}=\mathbf{0}$ remains nonvanishing in the thermodynamic limit. This proves BEC.

Reflection positivity is essential for our proof of BEC and forces the periodic potential to have period 2. Other generalizations can be accommodated, however, such as a more general lattice in which we add hopping to next-nearest neighbors [21] or the addition of nearest-neighbor interparticle repulsion [20]. For simplicity we concentrate here on the simple cubic lattice with on-site repulsion only.

In Sec. IV we show that the existence of BEC implies the absence of an energy gap for adding or removing a particle, and that the energy viewed as a function of the density has a unique tangent at $\varrho=\frac{1}{2}$, i.e., the chemical potential is continuous.

The absence of BEC for large λ or high temperatures T is proved in Sec. V. The technique applied here is a path space representation of the two-point function that follows from the Trotter product formula. This representation allows us to derive exponential decay of the two-point function, provided λ or T are sufficiently large, and hence absence of long-range order. The magnitude of λ or T enters through the suppression in the path space integral of long contours connecting a pair of lattice points if these parameters are large. The same representation is used for proving the existence of a gap, as explained in item (iii) in the Introduction. This method is quite robust and easily extends to a periodicity of the optical lattice potential different from 2, for instance.

In Sec. VI we show that the particle density (or 3-component of the spin) oscillates with the period of the staggered field if $\lambda \neq 0$, in contrast to the condensate wave function which is independent of λ and $\mathbf{x}$. For this effect the interaction is essential, as remarked in Sec. VII. Without the interaction there is *always* BEC (for low T) and the condensate wave function is *never* constant (for $\lambda \neq 0$).

In Appendix A, we shall prove that the ground state of (2) has total spin 0, which in the lattice gas language means that the lowest energy of (2) is obtained when the particle number is $|\Lambda|/2$. The essential ingredient in our proof is again reflection positivity of the Hamiltonian (2). We also show that the canonical partition function is maximal at half filling.

III. PROOF OF BEC FOR SMALL λ AND T

In this section we are going to show the occurrence of BEC for small λ and low enough temperature. The main result is the following.

THEOREM 1 (Existence of BEC). *Let* $E_{\mathbf{p}}=\sum_{i=1}^{d}[1-\cos(p_i)]$ *(where* p_i *denotes the components of* $\mathbf{p}$*) and*

$$c_d = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} d\mathbf{p} \frac{1}{E_{\mathbf{p}}}.$$

In the thermodynamic limit,

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda|^2} \sum_{\mathbf{x},\mathbf{y}\in\Lambda} \gamma(\mathbf{x},\mathbf{y}) \geq \frac{1}{2} - \frac{1}{2}\{\tfrac{1}{2}[d(d+1)+4\lambda^2]^{1/2} c_d\}^{1/2} - \frac{1}{\beta} c_d, \qquad (3)$$

with $\beta=1/(k_B T)$ *the inverse temperature. Moreover, if* $\varphi(\mathbf{x})$ *denotes the (normalized) eigenfunction corresponding to the largest eigenvalue of* $\gamma(\mathbf{x},\mathbf{y})$*, then* $\lim_{\Lambda\to\infty}|\Lambda|^{-1}|\Sigma_{\mathbf{x}}\varphi(\mathbf{x})|^2 = 1$*, implying that the condensate wave function is constant in the thermodynamic limit.*

Note that c_d is finite for $d \geq 3$. Since the largest eigenvalue of $\gamma(\mathbf{x},\mathbf{y})$ exceeds $|\Lambda|^{-1}\Sigma_{\mathbf{x},\mathbf{y}}\gamma(\mathbf{x},\mathbf{y})$, BEC is proved if the right side of the expression (3) is positive. This is in particular the case, for large enough β, as long as

$$\lambda^2 < \frac{1}{c_d^2} - \frac{d(d+1)}{4}.$$

In $d=3$, $c_3 \approx 0.505$ [20], and hence there is BEC for $\lambda \leq 0.960$. In Ref. [20] it was also shown that dc_d is monotone decreasing in d, which implies a similar result for all $d>3$.

The main tool in our proof of Theorem 1 is an infrared bound as in Ref. [20]. The statement is as follows. For A and B bounded linear operators, denote by

$$(A,B) = \int_0^1 \mathrm{Tr}\,(Ae^{-s\beta H}Be^{-(1-s)\beta H})ds/\mathrm{Tr}\,e^{-\beta H}$$

the Duhamel two-point function. For $\mathbf{p} \in \Lambda^*$ (the dual lattice), $\mathbf{p} \neq \mathbf{0}$ and $\widetilde{S}^1_{\mathbf{p}} = |\Lambda|^{-1/2}\Sigma_{\mathbf{x}} S^1_{\mathbf{x}} \exp(i\mathbf{p}\cdot\mathbf{x})$, we claim that

$$(\widetilde{S}^1_{\mathbf{p}}, \widetilde{S}^1_{-\mathbf{p}}) \leq \frac{1}{2\beta E_{\mathbf{p}}}. \qquad (4)$$

The same is true with $\widetilde{S}^1_{\mathbf{p}}$ replaced by $\widetilde{S}^2_{\mathbf{p}}$. This inequality will allow us to prove the bound (3) above. Moreover, we will infer from Eq. (4) the fact that there is only *one* large eigenvalue (of order $|\Lambda|$) of the one-particle density matrix, and the corresponding eigenfunction is constant (in the thermodynamic limit).

We start by proving Eq. (4). The main ingredient is

Gaussian domination. More precisely, let h be any real-valued function on Λ, and

$$Z(h) = \mathrm{Tr}\,\exp[-\beta K(h)],$$

where $K(h)$ is the modified Hamiltonian

$$K(h) = \sum_{\langle \mathbf{xy}\rangle} \left[\tfrac{1}{2}(S^1_{\mathbf{x}} - S^1_{\mathbf{y}} - h_{\mathbf{x}} + h_{\mathbf{y}})^2 - S^2_{\mathbf{x}} S^2_{\mathbf{y}}\right] + \lambda \sum_{\mathbf{x}} (-1)^{\mathbf{x}} S^3_{\mathbf{x}}.$$

Note that for $h=0$ this operator agrees with H up to a constant.

Lemma 1. *For all real-valued functions h,*

$$Z(h) \leqslant Z(0).$$

Proof. We perform a unitary transformation that takes $S^2 \mapsto -S^2$ and $S^3 \mapsto -S^3$ on the B sublattice. Since the trace does not change under unitary transformations, we have $Z(h) = \mathrm{Tr}\,\exp[-\beta \hat{K}(h)]$ with

$$\hat{K}(h) = \sum_{\langle \mathbf{xy}\rangle} \left[\tfrac{1}{2}(S^1_{\mathbf{x}} - S^1_{\mathbf{y}} - h_{\mathbf{x}} + h_{\mathbf{y}})^2 + S^2_{\mathbf{x}} S^2_{\mathbf{y}}\right] + \lambda \sum_{\mathbf{x}} S^3_{\mathbf{x}}.$$

Compared to $K(h)$, the sign in front of the $S^2_{\mathbf{x}} S^2_{\mathbf{y}}$ term has changed, and the $(-1)^{\mathbf{x}}$ has vanished. The operator $\hat{K}(h)$ thus obtained is translation invariant. Since S^1 and S^3 are real self-adjoint matrices, and S^2 is imaginary and self-adjoint, we meet exactly the conditions for applying the result in Ref. [20], Lemma 6.1 and proof of Theorem 4.2, to prove the lemma. ∎

The infrared bound (4) follows from this lemma by using the negativity of the second derivative,

$$\left.\frac{d^2}{d\varepsilon^2} Z(\varepsilon h)\right|_{\varepsilon=0} \leqslant 0.$$

By performing the derivative, we obtain

$$(A^\dagger, A) \leqslant \frac{1}{\beta} \sum_{\langle \mathbf{xy}\rangle} |h_{\mathbf{x}} - h_{\mathbf{y}}|^2,$$

where $A = \Sigma_{\langle \mathbf{xy}\rangle}(S^1_{\mathbf{x}} - S^1_{\mathbf{y}})(h_{\mathbf{x}} - h_{\mathbf{y}})$. We proved this inequality only for real-valued h, in which case $A = A^\dagger$, but it automatically extends in a standard way [20] to complex-valued h. In this case note that the adjoint of A agrees with its complex conjugate. Now, choosing $h_{\mathbf{x}} = \exp(i\mathbf{p}\cdot\mathbf{x})$, we obtain Eq. (4). By invariance of the Hamiltonian under rotations around the S^3 axis, the statement is also true with $\widetilde{S}^1_{\mathbf{p}}$ replaced by $\widetilde{S}^2_{\mathbf{p}}$.

We now want to use Ref. [20], Theorem 3.1, to relate the Duhamel two-point function to the ordinary thermal two-point function. For that purpose, we have to evaluate the double commutators

$$[\widetilde{S}^1_{\mathbf{p}}, [H, \widetilde{S}^1_{-\mathbf{p}}]] + [\widetilde{S}^2_{\mathbf{p}}, [H, \widetilde{S}^2_{-\mathbf{p}}]] = -\frac{2}{|\Lambda|}\left(H - \frac{1}{2}\lambda|\Lambda| + 2\sum_{\langle \mathbf{xy}\rangle} S^3_{\mathbf{x}} S^3_{\mathbf{y}} \cos\,\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})\right).$$

Let $C_{\mathbf{p}}$ denote the expectation value of this last expression,

$$C_{\mathbf{p}} = \langle [\widetilde{S}^1_{\mathbf{p}}, [H, \widetilde{S}^1_{-\mathbf{p}}]] + [\widetilde{S}^2_{\mathbf{p}}, [H, \widetilde{S}^2_{-\mathbf{p}}]]\rangle \geqslant 0.$$

The positivity of $C_{\mathbf{p}}$ can be seen from an eigenfunction expansion of the trace. From Ref. [20], Corollary 3.2 and Theorem 3.2, and Eq. (4) we infer that

$$\langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}}\rangle \leqslant \frac{1}{2}\sqrt{\frac{C_{\mathbf{p}}}{E_{\mathbf{p}}}} \coth \sqrt{\beta^2 C_{\mathbf{p}} E_{\mathbf{p}}/4}. \tag{5}$$

Using $\coth x \leqslant 1 + 1/x$ and Schwarz's inequality, we obtain for the sum over all $\mathbf{p} \neq \mathbf{0}$,

$$\sum_{\mathbf{p}\neq\mathbf{0}} \langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}}\rangle \leqslant \frac{1}{\beta}\sum_{\mathbf{p}\neq\mathbf{0}} \frac{1}{E_{\mathbf{p}}} + \frac{1}{2}\left(\sum_{\mathbf{p}\neq\mathbf{0}} \frac{1}{E_{\mathbf{p}}}\right)^{1/2} \left(\sum_{\mathbf{p}\neq\mathbf{0}} C_{\mathbf{p}}\right)^{1/2}.$$

We have $\Sigma_{\mathbf{p}\in\Lambda^*} C_{\mathbf{p}} = -2\langle H\rangle + \lambda|\Lambda|$, which can be bounded from above using the following lemma. Its proof follows exactly the same lines as Ref. [20], Theorem C.1.

Lemma 2. *The lowest eigenvalue of*

$$-\frac{1}{2} S^1_{\mathbf{x}} \sum_{i=1}^{2d} S^1_{\mathbf{y}_i} - \frac{1}{2} S^2_{\mathbf{x}} \sum_{i=1}^{2d} S^2_{\mathbf{y}_i} + \lambda S^3_{\mathbf{x}} \tag{6}$$

is given by $-\frac{1}{4}[d(d+1) + 4\lambda^2]^{1/2}$.

Since the Hamiltonian can be written as a sum of terms like (6), with $\mathbf{y}_i$ the nearest neighbors of $\mathbf{x}$, we get from this lemma the lower bound

$$H \geqslant -\frac{|\Lambda|}{4}[d(d+1) + 4\lambda^2]^{1/2} + \frac{1}{2}\lambda|\Lambda|.$$

With the aid of the sum rule

$$\sum_{\mathbf{p}\in\Lambda^*} \langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}}\rangle = \frac{|\Lambda|}{2}$$

[which follows from $(S^1)^2 = (S^2)^2 = 1/4$], we obtain a lower bound, in the thermodynamic limit,

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda|}\langle \widetilde{S}^1_{\mathbf{0}} \widetilde{S}^1_{\mathbf{0}} + \widetilde{S}^2_{\mathbf{0}} \widetilde{S}^2_{\mathbf{0}}\rangle \geqslant \frac{1}{2} - \frac{1}{2}\{\tfrac{1}{2}[d(d+1) + 4\lambda^2]^{1/2} c_d\}^{1/2} - \frac{1}{\beta} c_d. \tag{7}$$

The connection with Bose-Einstein condensation is as follows. Since H is real, also $\gamma(\mathbf{x},\mathbf{y})$ is real and we have

$$\gamma(\mathbf{x},\mathbf{y}) = \langle S^+_{\mathbf{x}} S^-_{\mathbf{y}}\rangle = \langle S^1_{\mathbf{x}} S^1_{\mathbf{y}} + S^2_{\mathbf{x}} S^2_{\mathbf{y}}\rangle.$$

Hence if $\varphi_0 = |\Lambda|^{-1/2}$ denotes the constant function,

$$\langle \varphi_0 | \gamma | \varphi_0\rangle = \langle \widetilde{S}^1_{\mathbf{0}} \widetilde{S}^1_{\mathbf{0}} + \widetilde{S}^2_{\mathbf{0}} \widetilde{S}^2_{\mathbf{0}}\rangle,$$

and thus the bound (7) implies Eq. (3). In addition we claim that the infrared bounds imply

$$\langle \xi | \gamma | \xi\rangle \leqslant \mathrm{const} \times |\Lambda|^{2/d} \tag{8}$$

for any normalized ξ that is orthogonal to φ_0, with a constant that is independent of ξ. It then follows easily that, with φ being the condensate wave function, $\lim_{\Lambda\to\infty} |\langle \varphi_0 | \varphi\rangle| = 1$, as claimed.

To prove Eq. (8) consider the positive definite matrix $\langle \tilde{S}^+_{\mathbf{p}} \tilde{S}^-_{-\mathbf{q}} \rangle$, with $\mathbf{p} \neq \mathbf{0}$, $\mathbf{q} \neq \mathbf{0}$. The infrared bound (5) implies that the diagonal of this matrix is bounded by $\langle \tilde{S}^+_{\mathbf{p}} \tilde{S}^-_{-\mathbf{p}} \rangle \leq \text{const} \times |\mathbf{p}|^{-2} \leq \text{const} \times |\Lambda|^{2/d}$ for $\mathbf{p} \neq \mathbf{0}$. Moreover, the matrix is almost diagonal in the sense that $\langle \tilde{S}^+_{\mathbf{p}} \tilde{S}^-_{-\mathbf{q}} \rangle \neq 0$ only if $q_i = p_i$ or $q_i = p_i \pm \pi$ (by invariance under translation by two lattice sites). The largest eigenvalue of such a matrix is bounded above by 2^d times the maximum on the diagonal, namely $2^d \text{const} \times |\Lambda|^{2/d} \ll |\Lambda|$. This proves our claim.

We conclude that $\gamma(\mathbf{x},\mathbf{y})$ has exactly *one* large eigenvalue, with corresponding eigenfunction equal to φ_0 as $|\Lambda| \to \infty$. I.e., the condensate wave function is constant. The infrared bounds imply, in fact, that this holds whenever there is BEC and not only in the parameter region where we establish the latter. The constancy of the condensate wave function is surprising and is not expected to hold for densities different from $\frac{1}{2}$, where particle-hole symmetry is absent. In contrast to the condensate wave function the particle density shows the staggering of the periodic potential. We show this in Sec. VI below. It also contrasts with the situation for zero interparticle interaction, as discussed in Sec. VII.

IV. NO CUSP, NO GAP

The system is in a Mott insulator state at zero temperature if a finite change in the chemical potential is required to change the particle number in the ground state. We refer to this as a gap in the chemical potential. More precisely, if E_k denotes the lowest energy of (2) restricted to the sector of $\frac{1}{2}|\Lambda| + k$ particles (which corresponds to $S^3_{\text{tot}} \equiv \Sigma_{\mathbf{x}} S^3_{\mathbf{x}} = k$ in the spin language), a gap means that, for all k,

$$E_{-k} + E_k - 2E_0 \geq c|k| \tag{9}$$

for some $c > 0$ independent of Λ and k. Note that particle-hole symmetry implies that $E_{-k} + E_k - 2E_0 = 2(E_{|k|} - E_0)$. Note also that the notion of a gap in this sense is distinct from that of a spectral gap at fixed particle number.

In the next section we prove Eq. (9) for sufficiently large λ. In this section we will show that whenever there is BEC then Eq. (9) fails. In fact, we will prove that

$$E_k - E_0 \leq \frac{c_k}{|\Lambda|} \tag{10}$$

for some k-dependent $c_k > 0$, which is independent of Λ, i.e., that Eq. (9) does not hold for finite k.

This, however, does not rule out the possibility that the macroscopic system still acts as an insulator. To show that this is, indeed, also not the case, we prove that Eq. (9) fails for macroscopic k as well. More precisely, we will show that the thermodynamic limit of the ground-state energy per site, $e_\infty(\varrho) = \lim_{\Lambda \to \infty} E_k/|\Lambda|$, where $k = (\varrho - \frac{1}{2})|\Lambda|$, satisfies a bound

$$0 \leq e_\infty(\varrho) - e_\infty\left(\tfrac{1}{2}\right) \leq \text{const} \times \left(\varrho - \tfrac{1}{2}\right)^2 \tag{11}$$

for ϱ close to 1/2, i.e., that there is no macroscopic cusp in the energy at half filling.

We will first prove Eq. (11). With $|0\rangle$ being the ground state of H, and with $\mathbf{y}$ some point in the lattice, consider the states

$$|\psi_{\mathbf{y}}\rangle = e^{i\varepsilon S^2_{\text{tot}}} \left(S^1_{\mathbf{y}} + \tfrac{1}{2}\right)|0\rangle.$$

The motivation is the following: we take the ground state and first project onto a given direction of S^1 on some site $\mathbf{y}$. If there is long-range order, this should imply that essentially all the spins point in this direction now. Then we rotate slightly around the S^2 axis. The particle number should then go up by $\varepsilon|\Lambda|$, but the energy only by $\varepsilon^2|\Lambda|$.

The norm of $|\psi_{\mathbf{y}}\rangle$ is given by

$$\langle \psi_{\mathbf{y}} | \psi_{\mathbf{y}} \rangle = \langle 0 | S^1_{\mathbf{y}} + \tfrac{1}{2} | 0 \rangle = \tfrac{1}{2},$$

where we used the symmetry $S^{1,2} \to -S^{1,2}$. We want to find an upper bound to the average energy of these states, more precisely,

$$\Delta E \equiv \frac{2}{|\Lambda|} \sum_{\mathbf{y}} \langle \psi_{\mathbf{y}} | H - E_0 | \psi_{\mathbf{y}} \rangle.$$

Here E_0 denotes the ground-state energy of H, which is obtained at half filling (see Appendix A). We claim that the inequality

$$e^{-i\varepsilon S^2_{\text{tot}}} H e^{i\varepsilon S^2_{\text{tot}}} \leq H + i\varepsilon [H, S^2_{\text{tot}}] + \text{const} \times \varepsilon^2 |\Lambda| \tag{12}$$

holds for some constant depending only on d and λ. To see this, consider, for self-adjoint operators A and C,

$$F_A(\varepsilon) = e^{i\varepsilon C} A e^{-i\varepsilon C}.$$

By Taylor's formula

$$F_A(\varepsilon) \leq F_A(0) + \varepsilon F'_A(0) + \frac{1}{2}\varepsilon^2 \sup_{0 \leq \eta \leq \varepsilon} \|F''_A(\eta)\|. \tag{13}$$

Note that the last norm is actually independent of η, since $e^{-i\varepsilon C}$ is unitary, and is given by the norm of the double commutator $[C,[C,A]]$. After evaluating the double commutator for the case in question, a simple bound gives Eq. (12).

Consider now the first term on the right side of Eq. (12). We obtain

$$\begin{aligned}
&\sum_{\mathbf{y}} \langle 0 | (S^1_{\mathbf{y}} + \tfrac{1}{2})(H - E_0)(S^1_{\mathbf{y}} + \tfrac{1}{2}) | 0 \rangle \\
&= \tfrac{1}{2} \sum_{\mathbf{y}} \langle 0 | [S^1_{\mathbf{y}}, [H, S^1_{\mathbf{y}}]] | 0 \rangle \\
&= \tfrac{1}{2} \langle 0 | \sum_{\langle \mathbf{xy} \rangle} 2 S^2_{\mathbf{x}} S^2_{\mathbf{y}} - \lambda \sum_{\mathbf{y}} (-1)^{\mathbf{y}} S^3_{\mathbf{y}} | 0 \rangle \\
&= -\tfrac{1}{2}(E_0 - \tfrac{1}{2}\lambda|\Lambda|),
\end{aligned}$$

where we used rotational symmetry in the last step. The second term,

$$\sum_{\mathbf{y}} \langle 0 | (S^1_{\mathbf{y}} + \tfrac{1}{2})[H, S^2_{\text{tot}}](S^1_{\mathbf{y}} + \tfrac{1}{2}) | 0 \rangle,$$

is zero by symmetry, as can be seen in the following way. The diagonal terms are zero by the symmetry $S^{1,2}_{\mathbf{x}} \to -S^{1,2}_{\mathbf{x}}$ at all sites. The off-diagonal terms are

$$\langle 0|S^1_{\rm tot}[H,S^2_{\rm tot}]+[H,S^2_{\rm tot}]S^1_{\rm tot}|0\rangle,$$

which is zero by the symmetry $S^{1,3}_{\mathbf{x}}\to -S^{1,3}_{\mathbf{x}}$ at all sites, followed by a unit-vector translation in any of the lattice directions. We therefore get that

$$\Delta E \leqslant \text{const}\times\varepsilon^2|\Lambda|+\frac{|E_0|+\frac{1}{2}\lambda|\Lambda|}{|\Lambda|}.$$

It remains to evaluate the average particle number of the states considered. Using that $S^3_{\rm tot}|0\rangle=0$, we obtain

$$\frac{2}{|\Lambda|}\sum_{\mathbf{y}}\langle 0|(S^1_{\mathbf{y}}+\tfrac{1}{2})e^{-i\varepsilon S^2_{\rm tot}}S^3_{\rm tot}e^{i\varepsilon S^2_{\rm tot}}(S^1_{\mathbf{y}}+\tfrac{1}{2})|0\rangle$$
$$=\frac{2}{|\Lambda|}\sin\varepsilon\,\langle 0|(S^1_{\rm tot})^2|0\rangle,$$

which is of the order $\varepsilon|\Lambda|$ if there is BEC. Choosing ε proportional to the chemical potential μ, we obtain as an upper bound for the ground-state energy of $H-\mu S^3_{\rm tot}$,

$$E_0(1-|\Lambda|^{-1})+\tfrac{1}{2}\lambda-c\mu^2|\Lambda|$$

for small μ, with $c>0$ in the case of BEC. By taking a Legendre transform, we arrive at Eq. (11).

To prove Eq. (10) we use as a trial state $(S^+_{\rm tot})^k|0\rangle$, with $k\geqslant 1$. Using the particle-hole symmetry of H as well as the fact that we are considering the ground state, we get the bound

$$E_k\leqslant E_0+\frac{1}{2}\frac{\langle[[(S^-_{\rm tot})^k,[H,(S^+_{\rm tot})^k]]\rangle}{\langle(S^-_{\rm tot})^k(S^+_{\rm tot})^k\rangle}.$$

Since there is BEC, $\langle(S^-_{\rm tot})^k(S^+_{\rm tot})^k\rangle\geqslant c'_k|\Lambda|^{2k}$ for some $c'_k>0$ modulo lower-order terms as $|\Lambda|\to\infty$. All we have to show is that $[(S^-_{\rm tot})^k,[H,(S^+_{\rm tot})^k]]\leqslant c''_k|\Lambda|^{2k-1}$ for some constant c''_k. This is clear, however, since altogether there are $|\Lambda|^{2k+1}$ factors, and the two commutators reduce the power by 2. Hence we obtain Eq. (10).

V. GAP FOR LARGE λ, AND ABSENCE OF BEC FOR LARGE λ OR HIGH TEMPERATURE

We shall now present explicit bounds for a region of values of (λ,T) for which BEC is absent. This region includes:

(i) all $\lambda\geqslant 0$ at $k_BT>d/(2\ln 2)$,

(ii) all $T\geqslant 0$ at $\lambda\geqslant 0$ such that $\lambda+|e(\lambda)|>d$.

The absolute (i.e., without specifying N) ground-state energy per site for a finite Λ, which is always obtained at half filling, is denoted by $e(\lambda)$. Note that $e(\lambda)<0$.

In this regime, the particles are localized in the sense that the transition amplitudes decay exponentially. Short excursions occur locally in "space-time"; however, a long-distance transition requires a linked chain, or percolation, of such local events and the amplitude for that decays exponentially, as in subcritical percolation models. One may discern here two distinct mechanisms contributing to the localization: at high λ localization is caused by the confinement due to the staggered structure of the potential, whereas at high temperatures it is a combined effect of the exclusion (no more than one particle at a lattice site) with the reduced amplitude for coordinated moves by neighboring particles. The above picture is made precise in a representation of the matrix elements of $e^{-\beta H}$ which in effect involves an "imaginary time."

There is a long history of rigorous results on quantum spin systems using a space-time approach to develop convergent expansions (see, for example, Ref. [22], especially Sec. 4). In this work we shall not utilize such expansions, and instead employ bounds which are derived from the basic loop-gas representation.

A more inclusive statement of the condition under which our results hold is

$$1-\frac{\lambda-f}{d}<e^{-(\lambda-f)\beta},\tag{14}$$

where $f\equiv f(\beta,\lambda)=-(\beta|\Lambda|)^{-1}\ln\operatorname{Tr}e^{-\beta H}$ is the free energy per site, which satisfies

$$-f(\beta,\lambda)\geqslant\max\left\{|e(\lambda)|,\beta^{-1}\ln 2-\frac{1}{2}\lambda\right\}.$$

Under condition (14), we define $\nu>0$ by

$$e^{-\nu}\equiv\frac{d}{\lambda-f}(1-e^{-\beta(\lambda-f)})<1.$$

THEOREM 2 (Mott insulator phase). *Throughout the regime where Eq. (14) holds the thermal average two-point function decays exponentially. More specifically, for any* $\xi<\nu$

$$\gamma(\mathbf{x},\mathbf{y})=\frac{\operatorname{Tr}a^\dagger_{\mathbf{x}}a_{\mathbf{y}}e^{-\beta H}}{\operatorname{Tr}e^{-\beta H}}\leqslant C_\xi\,e^{-\xi|\mathbf{x}-\mathbf{y}|}\tag{15}$$

with $C_\xi=[1-e^{\xi-\nu}]^{-1}$. *Similar decay also holds in the finite volume ground state [corresponding to the limit* $\beta\to\infty$ *in Eq. (15)].*

Moreover, the ground-state energy E_k *for particle number* $\frac{1}{2}|\Lambda|+k$ *satisfies*

$$E_k+E_{-k}-2E_0=2(E_k-E_0)\geqslant c|k|,\tag{16}$$

with $c=2[\lambda+|e(\lambda)|-d]$, *which is strictly positive for large* λ *(independently of the volume* $|\Lambda|$*).*

Equation (16) is, in fact, the consequence of a more explicit result: If $\mathcal{P}_k$ denotes the projection onto the subspace of fixed particle number $N=\frac{1}{2}|\Lambda|+k$, then

$$\frac{\operatorname{Tr}\mathcal{P}_ke^{-\beta H}}{\operatorname{Tr}\mathcal{P}_0e^{-\beta H}}\leqslant 2\,e^{-\alpha\beta|k|}\left[\frac{e^2}{1-B(\alpha)}\frac{|\Lambda|}{|k|}\right]^{|k|},\tag{17}$$

for any $\alpha>0$ for which

$$B(\alpha)\equiv d\int_0^\beta e^{-[\lambda+|f_0(\beta,\lambda)|-\alpha]t}dt<1,$$

with $f_0(\beta,\lambda)$ denoting the free energy (per site) for the system with fixed particle number $N=|\Lambda|/2$. Equation (16) is

derived by considering the leading terms in Eq. (17) in the limit $\beta\to\infty$ at fixed Λ. In the thermodynamic limit Eq. (16) means that, in contrast to Eqs. (10) and (11), the energy per site, $e_\infty(\varrho)$, has a cusp at $\varrho=1/2$, and hence (by Legendre transform) the half filled state $\varrho=1/2$ corresponds to a whole interval of values for the chemical potential.

For nonzero temperature the energy dependence on k may show some rounding due to thermal excitations; however, there is a cusp in the energy per site, when this function is viewed on a scale in which $|k|/|\Lambda|\geq e^{-r\beta c}$, with some $r<1$.

Theorem 2 is derived using a representation for the matrix elements of the relevant operators in the basis that diagonalizes $\{S^3_{\mathbf{x}}\}$. An important fact here is that the matrix elements of $e^{-\beta H}$ are positive in this basis. We write $H=H_0+\lambda W$ with H_0 the hopping term. The matrix elements can be expressed via the Dyson series

$$e^{t(A+B)}=e^{tA}\sum_{n\geq 0}\int_{0\leq t_1\leq t_2\leq\cdots\leq t} B(t_n)\cdots B(t_1)dt_1\cdots dt_n \quad (18)$$

with $B(t)=e^{-tA}Be^{tA}$. We apply this with $t=\beta$, $B=-H_0$, $A=-\lambda W$. This yields a functional-integral representation in terms of integrals over space-time configurations, which are represented below by ω. The resulting functional integral is not only positive, but also reflection positive, and we make use of that fact. However, reflection positivity is not essential for the qualitative picture, as even without it we would obtain similar results with only slightly weaker bounds—with f replaced by 0.

The measure space over which the integration takes place is a Cartesian product of the set of initial spin configurations times the space of configurations of "rungs," linking pairs of neighboring space-time sites. A rung is parametrized by a pair $\{\mathbf{x},\mathbf{y}\}$ of neighboring lattice sites and $t\in[0,\beta]$. For the matrix elements of $e^{-\beta H}$ between states which correspond to a pair of specified spin configurations, one naturally finds an integral over configurations of arbitrary number of rungs, over which we integrate with an "ideal-gas"-like measure, in which n-tuples are summed and integrated over with the weights $(z^n/n!)dt_1\cdots dt_n$. Each rung represents a transformation of the spin configuration affected by a specific term in the Hamiltonian, and the fugacity-like parameter z is the corresponding amplitude, which in the case of the Hamiltonian considered here, i.e., the hopping term H_0, is $z=1/2$.

It is particularly convenient to express the spin, or particle, configuration in terms of the timelines of the "quasiparticles" which are defined through the occupation numbers $n_{\mathbf{x}}=\frac{1}{2}+(-1)^{\mathbf{x}}S^3_{\mathbf{x}}$. There are no quasiparticles in the configuration that minimizes the potential energy, i.e., if there are $\frac{1}{2}|\Lambda|$ particles that sit on the B sublattice. The presence of a quasiparticle means either the presence of a particle ($S^3=+1/2$), if the site is even (A sublattice), or the absence of one ($S^3=-1/2$), if the site is odd (B sublattice). It is easy to check that in this representation the operators $a^\dagger_{\mathbf{x}}$ and $a_{\mathbf{x}}$ act as insertion of a source and, correspondingly, sink of excess spin (relative to the potential-minimizing configuration), although the direction in which the excess spin propagates changes with the parity of $\mathbf{x}$. Namely, creation of a particle on an A site (or annihilation on a B site) results in a quasiparticle running "upward in time," whereas a quasiparticle running "downward in time" originates from annihilation of a particle on an A site (or creation on a B site).

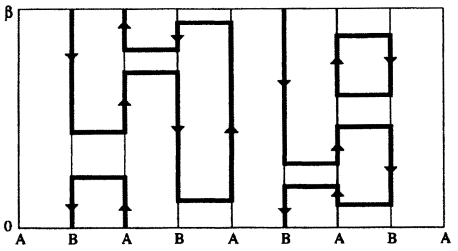

FIG. 2. Loop gas describing paths of quasiparticles for particle number $N=|\Lambda|/2-1$. A line on an A site means presence of a particle, while on a B site it means absence. The horizontal rungs correspond to hopping of a particle.

Proceeding along the above lines, as explained in greater detail in Ref. [23], one obtains

$$\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}=\int \upsilon_{1/2}(d\omega)e^{-\lambda|\omega|}I[\nu(\omega)=k], \quad (19)$$

where ω represents a configuration of a family of disjoint oriented loops in $\Lambda\times[0,\beta]$, defined with periodic boundary conditions in "time" ($[0,\beta]$), whose orientation alternates with $\mathbf{x}$, being "up" along A sites and "down" along B sites. For each configuration, $|\omega|$ is the total "vertical" length of the time lines in ω, and $\nu(\omega)$ is the total winding number in the periodic time direction. The indicator function $I[\nu(\omega)=k]$ is 1 if the loop configuration ω has total winding number k, and 0 otherwise. The winding number can also be computed by adding the spin orientations of the sites occupied by quasiparticles, along any "constant time" cut through the diagram. The measure $\upsilon_z(d\omega)$ corresponds to integration, with weights zdt, over the times at which the jumps to neighboring lattice sites occur, and summation over the possible numbers of such jumps. In effect, as mentioned above, the integral is over an ideal-gas-like distribution of the horizontal rungs in the diagram depicted in Fig. 2 with the fugacity parameter taking here the value $z=1/2$. That value is dictated by the Hamiltonian, where one finds $1/2$ in front of the "hopping term" $S^+_{\mathbf{x}}S^-_{\mathbf{y}}$. For later use, we find it convenient to consider the measures $\upsilon_z(d\omega)$ for general $z>0$, not only $z=1/2$.

Likewise, for $\mathbf{x}\neq\mathbf{y}$,

$$\mathrm{Tr}\,a^\dagger_{\mathbf{x}}a_{\mathbf{y}}\mathcal{P}_k e^{-\beta H}=\int_{\partial\omega=\delta_{(\mathbf{x},0)}-\delta_{(\mathbf{y},0)}} \upsilon_{1/2}(d\omega)e^{-\lambda|\omega|}\,I[\nu(\omega)=k], \quad (20)$$

where $\partial\omega$ is the set of sources of ω. More precisely, the configurations that contribute to the last integral have exactly *one* curve starting at $\mathbf{x}$ and ending at $\mathbf{y}$, both at time 0, for which we shall use the symbol γ, and otherwise only closed

loops, of the kind which appear in the corresponding trace without the source/sink operators.

Denoting by $\mathcal{A}^{\circ}$ the set of configurations ω that consist only of loops, i.e., closed curves, and by $\mathcal{A}^{(\mathbf{x},\mathbf{y})}$ the set of configurations containing one curve connecting $\mathbf{x}$ with $\mathbf{y}$ (at time 0) and otherwise only closed curves, the above representation yields for the thermal average unconstrained by the particle number

$$\langle S^{+}_{\mathbf{x}} S^{-}_{\mathbf{y}} \rangle = \frac{\int_{\mathcal{A}^{(\mathbf{x},\mathbf{y})}} \upsilon_{1/2}(d\omega) e^{-\lambda|\omega|}}{\int_{\mathcal{A}^{\circ}} \upsilon_{1/2}(d\omega) e^{-\lambda|\omega|}}. \tag{21}$$

Now let $\mathcal{B}^{(\mathbf{x},\mathbf{y})} \subset \mathcal{A}^{(\mathbf{x},\mathbf{y})}$ denote the set of ω's which consist of exactly *one* curve connecting $\mathbf{x}$ and $\mathbf{y}$, no other curves. For a collection of disjoint curves $\{\gamma_j\}$, let $\mathcal{A}^{\circ}_{\{\gamma_j\}} \subset \mathcal{A}^{\circ}$ denote the set of ω's that avoid the collection $\{\gamma_j\}$ or, in other words, that are consistent with it in the sense that insertion of the curves into ω would still give an admissible configuration of nonintersecting curves. The measures $\upsilon_z(d\omega)$ obviously have the product structure

$$\int_{\mathcal{A}^{(\mathbf{x},\mathbf{y})}} \upsilon_z(d\omega) e^{-\lambda|\omega|} = \int_{\mathcal{B}^{(\mathbf{x},\mathbf{y})}} \upsilon_z(d\gamma) e^{-\lambda|\gamma|} \int_{\mathcal{A}^{\circ}_{\gamma}} \upsilon_z(d\omega) e^{-\lambda|\omega|},$$

where we identified ω with γ in the first integral on the right. The following is a convenient bound on the last factor.

Lemma 3 (Contour bound). *For any family of disjoint curves* $\{\gamma_j\}$,

$$\int_{\mathcal{A}^{\circ}_{\{\gamma_j\}}} \upsilon_z(d\omega) e^{-\lambda|\omega|} \leq e^{\Sigma_j |\gamma_j| f} \int_{\mathcal{A}^{\circ}} \upsilon_z(d\omega) e^{-\lambda|\omega|}, \tag{22}$$

where f is the free energy per site. Furthermore, a similar bound holds for the integrals further restricted by the condition $I[\nu(\omega)=0]$ and f replaced by f_0 [which equals $-(\beta|\Lambda|)^{-1}\ln \mathrm{Tr}\, \mathcal{P}_0 e^{-\beta H}$].

The proof, which is presented in Appendix B, uses the chessboard inequality, which is a consequence of the reflection positivity of the functional integral. As was mentioned already, our main qualitative conclusions do not require this result, and would follow already from the trivial bound in which f and f_0, which satisfy $f<f_0<0$, are replaced by 0.

Lemma 3 implies that

$$\langle S^{+}_{\mathbf{x}} S^{-}_{\mathbf{y}} \rangle \leq \int_{\mathcal{B}^{(\mathbf{x},\mathbf{y})}} \upsilon_{1/2}(d\gamma) e^{-|\gamma|(\lambda - f)}. \tag{23}$$

To evaluate such expressions, it is useful to consider the quantity

$$\chi(z,\lambda) = \sup_{\hat{x},\hat{y}} \int_{\mathcal{B}^{(\hat{x},\hat{y})}} \upsilon_z(d\gamma) e^{-\lambda|\gamma|},$$

where $\hat{x}=(\mathbf{x},t_x)$ and $\hat{y}=(\mathbf{y},t_y)$ are arbitrary points in $\Lambda \times [0,\beta]$.

Lemma 4. *If* $2zd\int_0^{\beta} e^{-\lambda t} dt < 1$, *then*

$$\chi(z,\lambda) \leq \frac{1}{1 - 2zd\int_0^{\beta} e^{-\lambda t} dt}. \tag{24}$$

Furthermore, for any $\{\hat{x},\hat{y}\}$ *and* $\xi,\alpha>0$,

$$\begin{aligned} \int_{\mathcal{B}^{(\hat{x},\hat{y})}} \upsilon_z(d\gamma) e^{-\lambda|\gamma|} &\leq e^{-\xi|\mathbf{x}-\mathbf{y}|} \chi(ze^{\xi},\lambda), \\ \int_{\mathcal{B}^{(\hat{x},\hat{y})}} \upsilon_z(d\gamma) e^{-\lambda|\gamma|} I[|\gamma| \geq t] &\leq e^{-\alpha t} \chi(z,\lambda-\alpha). \end{aligned} \tag{25}$$

Proof. The first inequality here is a random walk bound, which is derived by the following "renewal-type" argument: split the integral into a part that comes from curves that do not jump at all (which only occurs if $\mathbf{x}=\mathbf{y}$) and a part where γ has at least one jump. The contribution from the path that does not jump is at most 1. The first jump can be in $2d$ possible directions, hence one gets

$$\chi \leq 1 + 2zd\int_0^{\beta} e^{-\lambda t} dt\, \chi.$$

Since in a finite volume $\chi<\infty$ *a priori*, this yields Eq. (24).

The rest follows by fairly direct arguments, noting that $\upsilon_{ze^{\xi}}(d\gamma) = \upsilon_z(d\gamma) e^{\xi \#(\gamma)}$, where $\#(\gamma)$ denotes the number of jumps of γ, which is greater or equal to $|\mathbf{x}-\mathbf{y}|$ in the case in question. The second inequality in (25) is obtained by estimating $I[|\gamma| \geq t] \leq e^{\alpha(|\gamma|-t)}$ for any positive α. ∎

We shall now use the above functional representation to derive Theorem 2.

By applying the bounds (23)–(25) to the random-walk representation (21), we see that under the condition stated in Eq. (14) the two-point function decays exponentially, as claimed in Eq. (15).

To prove Eq. (17) we start by noting that in case $N \neq |\Lambda|/2$ the integral in Eq. (19) is over configurations with a nontrivial winding number, $\nu(\omega)=k$. Each such configuration includes a collection of "noncontractible" loops $\{\gamma_j\}$ with nonzero winding numbers, $\nu_j \equiv \nu(\gamma_j) \neq 0$. The total length of the set $\{\gamma_j\}$ is at least $\beta|k|$. We shall bound the relative weight of such configurations by using the second bound in (25) and combining it with an argument whose purpose is to control the "entropy" of such a collection of long loops.

Each noncontractible loop γ_j can be labeled by a starting point $\mathbf{x}_j \in \Lambda$ where γ_j crosses the 0 time line, and a winding number ν_j. We shall actually overcount by summing over all possible $\mathbf{x}_j$'s as starting points for the loops (with the only restriction that $\mathbf{x}_j \neq \mathbf{x}_i$ for $j \neq i$), and over all possible winding numbers ν_j with $\Sigma_j |\nu_j| \geq |k|$.

For a given collection $\{\gamma_j\}$ of noncontractible loops, we can bound the integral over the remaining loops by an integral over loops with zero total winding number that avoid the γ_i's. Hence, starting from Eq. (19), we get the bound

$$\frac{\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathcal{P}_0 e^{-\beta H}} \leq \sum_{\{\mathbf{x}_1,\mathbf{x}_2,\ldots\}\subset\Lambda} \times\prod_j \int_{B^c(\mathbf{x}_j,\mathbf{x}_j)} v_{1/2}(d\gamma_j) e^{-\lambda|\gamma_j|} I[\nu(\gamma_j)\neq 0] \times I\Big[\sum_j |\nu(\gamma_j)| \geq |k|\Big] I_{\mathrm{ni}}[\{\gamma_1,\gamma_2,\ldots\}] \times \frac{\int_{\mathcal{A}^o_{\{\gamma_j\}}} v_{1/2}(d\omega) e^{-\lambda|\omega|} I[\nu(\omega)=0]}{\int_{\mathcal{A}^o} v_{1/2}(d\omega) e^{-\lambda|\omega|} I[\nu(\omega)=0]}.$$

Here I_{ni} denotes the indicator function for having only *non-intersecting* loops. Using the chessboard bound of Lemma 3, the last fraction can be bounded above by $\Pi_j e^{f_0(\beta,\lambda)|\gamma_j|}$, with $f_0(\beta,\lambda)<0$ the free energy per site at $N=|\Lambda|/2$. Applying the bounds of Lemma 4 to the integral over n loops γ_i with given absolute value of the winding number, $m_i=|\nu_i|$, we have, for any $\alpha>0$,

$$\prod_{j=1}^{n} \int_{B^c(\mathbf{x}_j,\mathbf{x}_j)} v_{1/2}(d\gamma_j) e^{-(\lambda+|f_0|)|\gamma_j|} I[|\nu(\gamma_j)|=m_j] \leq \hat{\chi}(\alpha)^n e^{-\alpha\beta\Sigma_j m_j}. \tag{26}$$

Here $\hat{\chi}(\alpha)=\chi(1/2,\lambda+|f_0(\beta,\lambda)|-\alpha)$, which is finite if α is not too large.

To complete the bound, we have to sum the right side of Eq. (26) over all the possible choices of the collection of the starting points of the winding loops $\{\mathbf{x}_1,\ldots,\mathbf{x}_n\}$, and over all possible winding numbers ν_j with $|\nu_j|>1$ and $\Sigma_j|\nu_j|\geq|k|$. To do so, we employ the following device. Defining

$$P(z)=1+\hat{\chi}(\alpha)\sum_{i=1}^{|\Lambda|/2}(z\delta)^i,$$

with $\delta=e^{-\alpha\beta}$, we see that the sum in question is given by the sum of all the coefficients of z^l in $P(z)^{|\Lambda|}$ with powers $l\geq|k|$. Hence

$$\frac{\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathcal{P}_0 e^{-\beta H}} \leq \frac{1}{2\pi i}\oint_{|z|=R} \frac{dz}{z^{|k|+1}} \frac{1}{1-z^{-1}} P(z)^{|\Lambda|},$$

where R can be any number greater than 1. The contour integral serves as a filter, selecting for us the relevant coefficients of the polynomial $P(z)^{|\Lambda|}$. A simple bound shows that the above quantity is bounded from above by

$$\inf_{1<R<1/\delta} \frac{1}{1-R^{-1}} \frac{e^{|\Lambda|\hat{\chi}(\alpha)[R\delta/(1-R\delta)]}}{R^{|k|}}.$$

We now choose $R=k/[\delta\hat{\chi}(\alpha)|\Lambda|]$, assuming that this quantity is greater or equal to 2. Note that $\delta R\leq\frac{1}{2}$, since $|k|\leq\frac{1}{2}|\Lambda|$ and $\hat{\chi}(\alpha)\geq 1$. Hence we obtain

$$\frac{\mathrm{Tr}\,\mathcal{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathcal{P}_0 e^{-\beta H}} \leq 2\, e^{-\alpha\beta|k|}\left[e^2\hat{\chi}(\alpha)\frac{|\Lambda|}{|k|}\right]^{|k|}.$$

This inequality is also valid, however, if $|k|/[\delta\hat{\chi}(\alpha)|\Lambda|]<2$, since the resulting bound then exceeds 1, which is greater than the left-hand side (as shown in Appendix A). This proves the claim made in Eq. (17), which presents sufficient conditions for the existence of a cusp in the energy dependence on N, i.e., of a gap in the chemical potential.

VI. NONCONSTANCY OF THE DENSITY

In Sec. III above we have demonstrated the existence of BEC for small λ and T, and also that the condensate wave function is constant. Despite this fact the particle density has the periodicity of the external potential and is not constant for $\lambda\neq 0$. More precisely, the following result is proved below.

THEOREM 3 (Nonconstancy of the density). *Let $\varrho(\mathbf{x})=\gamma(\mathbf{x},\mathbf{x})$ denote the particle density in the thermal equilibrium state at inverse temperature β. With $e(\lambda,\beta)=|\Lambda|^{-1}\langle H\rangle$ equal to the energy per site,*

$$\frac{1}{|\Lambda|}\left|\sum_{\mathbf{x}\in\Lambda}(-1)^{\mathbf{x}}\varrho(\mathbf{x})\right| \geq \frac{\lambda|e(0,\beta)|^2}{2d^2(3d+\lambda)}. \tag{27}$$

We first prove this for the ground state. We will show that the ground-state energy of H, denoted by $E(\lambda)$, satisfies

$$E(\lambda)\leq E(0)+\tfrac{1}{2}\lambda|\Lambda|-c\lambda^2|\Lambda|, \tag{28}$$

with $c=\frac{1}{2}e_0^2d^{-2}/(3d+\lambda)$. [Here $e_0=E(0)/|\Lambda|$ denotes the ground-state energy per site at $\lambda=0$.] Equation (28) implies Eq. (27) by the following argument. Write $H=H_0+\lambda W$, with the obvious notation for H_0 and W. Since $E(\lambda)$ is a concave function of λ, we have

$$\langle W\rangle=E'(\lambda)\leq\frac{E(\lambda)-E(0)}{\lambda}\leq\frac{1}{2}|\Lambda|-c\lambda|\Lambda|.$$

On the other hand,

$$\langle W\rangle=\sum_{\mathbf{x}\in\Lambda}\left[\frac{1}{2}+(-1)^{\mathbf{x}}\langle S^3_{\mathbf{x}}\rangle\right]=\frac{1}{2}|\Lambda|+\sum_{\mathbf{x}\in\Lambda}(-1)^{\mathbf{x}}\varrho(\mathbf{x}).$$

Combining the last two equations, we obtain

$$\frac{1}{|\Lambda|}\left|\sum_{\mathbf{x}\in\Lambda}(-1)^{\mathbf{x}}\varrho(\mathbf{x})\right|\geq c\lambda,$$

which proves our claim.

It remains to show Eq. (28). To do this, let the operator C be given by

$$C=\frac{1}{2}\sum_{\langle\mathbf{xy}\rangle}(-1)^{\mathbf{x}}(S^1_{\mathbf{x}}S^2_{\mathbf{y}}-S^2_{\mathbf{x}}S^1_{\mathbf{y}}).$$

As in the Hamiltonian, the sum is over all nearest-neighbor pairs, each pair counted only once. This operator has the nice property that

$$[C,W]=iH_0.$$

Proceeding as in Eqs. (12) and (13), a simple bound of the relevant double commutators gives

$$e^{i\varepsilon C}We^{-i\varepsilon C}\leq W-\varepsilon H_0+\varepsilon^2\frac{d^2}{2}|\Lambda|$$

as well as

$$e^{i\varepsilon C}H_0e^{-i\varepsilon C}\leq H_0+i\varepsilon[C,H_0]+\varepsilon^2\frac{3d^3}{2}|\Lambda|.$$

Note that the ε^2 terms are of order of the volume, due to the fact that both C and H contain only nearest-neighbor terms. With $|0\rangle$ the ground state of H_0, we therefore have, using $\langle 0|W|0\rangle=\frac{1}{2}|\Lambda|$ and $\langle 0|[C,H_0]|0\rangle=0$,

$$\begin{aligned}E(\lambda)&\leq\langle 0|e^{i\varepsilon C}He^{-i\varepsilon C}|0\rangle\\&\leq E(0)(1-\varepsilon\lambda)+\tfrac{1}{2}\lambda|\Lambda|+\tfrac{1}{2}\varepsilon^2d^2(3d+\lambda)|\Lambda|.\end{aligned}$$

Now the optimal choice of ε is $\varepsilon=2c\lambda/e_0$, which finishes the proof of Eq. (28).

A similar argument works at positive temperature. It shows that the free energy depends nontrivially on λ, and by the same concavity argument as above this implies the nonconstancy of the density, also at positive temperature, as claimed in Eq. (27).

VII. THE NONINTERACTING GAS

The interparticle interaction is essential for the existence of a Mott insulator phase for large λ. In case of absence of the hard-core interaction, there is BEC for any density and any λ at low enough temperature (for $d\geq 3$). To see this, we have to calculate the spectrum of the one-particle Hamiltonian $-\frac{1}{2}\Delta+V(\mathbf{x})$, where Δ denotes the discrete Laplacian and $V(\mathbf{x})=\lambda(-1)^{\mathbf{x}}$. The spectrum can be easily obtained by noting that V anticommutes with the off-diagonal part of the Laplacian, i.e., $\{V,\Delta+2d\}=0$. Hence

$$\left[-\frac{1}{2}\Delta-d+V(\mathbf{x})\right]^2=\left(-\frac{1}{2}\Delta-d\right)^2+\lambda^2,$$

so the spectrum is given by

$$d\pm\sqrt{(\textstyle\sum_i\cos p_i)^2+\lambda^2},$$

where $\mathbf{p}\in\Lambda^*$. In particular, $E(\mathbf{p})-E(0)\sim\frac{1}{2}d(d^2+\lambda^2)^{-1/2}|\mathbf{p}|^2$ for small $|\mathbf{p}|$, and hence there is BEC for low enough temperature. Note that the condensate wave function is of course not constant in this case, but rather given by the eigenfunction corresponding to the lowest eigenvalue of $-\frac{1}{2}\Delta+\lambda(-1)^{\mathbf{x}}$.

VIII. CONCLUSION

We have introduced a lattice model, which is similar to the usual Bose-Hubbard model and which describes the transition between Bose-Einstein condensation and a Mott insulator state as the strength λ of the optical lattice potential is increased. While the model is not soluble in the usual sense, we can prove rigorously all the essential features that are observed experimentally. These include the existence of BEC for small λ and its suppression for large λ, which is a localization phenomenon depending heavily on the fact that the Bose particles interact with each other. In the Mott insulator regime we prove the existence of a gap in the chemical potential, which does not exist in the BEC phase and for which the interaction is also essential. Bounds on the critical λ as a function of temperature are included.

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APPENDIX A: HALF FILLING AND REFLECTION POSITIVITY

In this appendix we will show that H has a *unique* ground state which has particle number $|\Lambda|/2$. For $\lambda=0$, this was previously shown in Ref. [24]. We also establish the corresponding result at positive temperature, namely that the canonical partition function is maximal for particle number $N=|\Lambda|/2$, although we do not prove that the maximum is obtained only at half filling.

The operator H commutes with $\Sigma_{\mathbf{x}}S^3_{\mathbf{x}}$. By a Perron-Frobenius argument the ground state of H restricted to the subspace with fixed value of $\Sigma_{\mathbf{x}}S^3_{\mathbf{x}}$ is unique. We claim that the absolute ground state of H corresponds to the value $\Sigma_{\mathbf{x}}S^3_{\mathbf{x}}=0$. To prove this we shall use reflection positivity.

We divide the lattice into a left part and a right part $\Lambda=\Lambda_L\cup\Lambda_R$ of equal size. We shall identify the space $\mathcal{H}_1=\otimes_{\mathbf{x}\in\Lambda_L}\mathbb{C}^2$ with the space $\otimes_{\mathbf{x}\in\Lambda_R}\mathbb{C}^2$, by identifying factors reflected in the middle plane. We may therefore write the total Hilbert space as $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_1$. We may then write

$$H=H_L\otimes I+I\otimes H_R-\frac{1}{2}\sum_{\langle\mathbf{xy}\rangle\in M}(S^+_{\mathbf{x}}S^-_{\mathbf{y}}+S^-_{\mathbf{x}}S^+_{\mathbf{y}}),$$

where H_L and H_R act on $\mathcal{H}_1$ and M denotes the set of bonds going from the left sublattice to the right sublattice (note that because of the periodic boundary condition these include the bonds that connect the right boundary with the left boundary). Note that $H_L\neq H_R$.

We now change H to the unitarily equivalent operator H' for which at all sites on the right sublattice we change $S^{\pm}_{\mathbf{x}}\to S^{\mp}_{\mathbf{x}}$ and $S^3_{\mathbf{x}}\to -S^3_{\mathbf{x}}$. We have

$$H'=H_L\otimes I+I\otimes H_L-\frac{1}{2}\sum_{\langle\mathbf{xy}\rangle\in M}(S^+_{\mathbf{x}}S^+_{\mathbf{y}}+S^-_{\mathbf{x}}S^-_{\mathbf{y}}).$$

The same unitary will change $\Sigma_{\mathbf{x}}S^3_{\mathbf{x}}$ to $S'=S\otimes I-I\otimes S$, where $S=\Sigma_{\mathbf{x}\in\Lambda_L}S^3_{\mathbf{x}}$ acts on $\mathcal{H}_1$.

Let $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_1$ be a normalized absolute ground state for H' with $S'|\psi\rangle = m|\psi\rangle$. We want to show that $m=0$. We may write $|\psi\rangle = \Sigma_n |\psi_n\rangle$, where $S \otimes I|\psi_n\rangle = n|\psi_n\rangle$ and $I \otimes S|\psi_n\rangle = (n-m)|\psi_n\rangle$.

We may consider any state $|\phi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_1$ as an operator from the Hilbert space $\mathcal{H}_1$ to itself, in the following way. We introduce a basis $|X\rangle$ in $\mathcal{H}_1$ indexed by subsets $X \subseteq \Lambda_L$, labeling the state with all spins up at the sites in X and down elsewhere. We shall refer to this representation as the standard basis. Then $|\phi\rangle$ may be represented as a function associating a complex number $\phi(X,Y)$ to any pair of subsets $X, Y \subseteq \Lambda_L$, namely $\phi(X,Y)$ is given by the inner product of $|X\rangle \otimes |Y\rangle$ with $|\phi\rangle$. Hence $|\phi\rangle$ may be identified with the operator $\hat{\phi}$ defined by the matrix elements $\langle X|\hat{\phi}|Y\rangle = \phi(X,Y)$.

If A is an operator on $\mathcal{H}_1$ then $\widehat{A \otimes I|\psi\rangle} = A\hat{\psi}$ and $\widehat{I \otimes A|\psi\rangle} = \hat{\psi}A^T$ where A^T is the *transposed* operator represented by the matrix $A^T(X,Y) = A(Y,X)$ in the standard basis. (Note that transposition is not a canonical operation, but depends on the basis in which it is defined.)

The operator S is represented by a real symmetric matrix in the standard basis. Thus in the above representation $\hat{\psi}_n$ maps the subspace where $S=(n-m)$ to the subspace where $S=n$ and vanishes on the orthogonal complement. Hence we see that $\hat{\psi}^\dagger\hat{\psi} = \Sigma_n \hat{\psi}_n^\dagger \hat{\psi}_n$ and likewise $\hat{\psi}\hat{\psi}^\dagger = \Sigma_n \hat{\psi}_n \hat{\psi}_n^\dagger$. It follows from this that $S\hat{\psi}^\dagger\hat{\psi} = \hat{\psi}^\dagger\hat{\psi}S$ and $S\hat{\psi}\hat{\psi}^\dagger = \hat{\psi}\hat{\psi}^\dagger S$. Hence

$$S(\hat{\psi}^\dagger\hat{\psi})^{1/2} = (\hat{\psi}^\dagger\hat{\psi})^{1/2}S, \quad S(\hat{\psi}\hat{\psi}^\dagger)^{1/2} = (\hat{\psi}\hat{\psi}^\dagger)^{1/2}S. \quad \text{(A1)}$$

Let $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_1$ denote the states such that $\hat{\psi}_1 = (\hat{\psi}\hat{\psi}^\dagger)^{1/2}$ and $\hat{\psi}_2 = (\hat{\psi}^\dagger\hat{\psi})^{1/2}$. Then $|\psi_1\rangle$ and $|\psi_2\rangle$ are normalized [since $\langle\psi_1|\psi_1\rangle = \mathrm{Tr}(\hat{\psi}_1^\dagger\hat{\psi}_1) = \mathrm{Tr}(\hat{\psi}\hat{\psi}^\dagger) = \langle\psi|\psi\rangle$] and Eq. (A1) implies that $S'|\psi_1\rangle = 0$ and $S'|\psi_2\rangle = 0$.

We shall prove that

$$\langle\psi|H'|\psi\rangle \geq \frac{1}{2}\langle\psi_1|H'|\psi_1\rangle + \frac{1}{2}\langle\psi_2|H'|\psi_2\rangle. \quad \text{(A2)}$$

Since $|\psi\rangle$ is an absolute ground state we see that $|\psi_1\rangle$ and $|\psi_2\rangle$ are also absolute ground states. Since they both have $S'=0$ and the ground state with this property is unique we conclude that $|\psi_1\rangle = |\psi_2\rangle$, i.e., $\hat{\psi}^\dagger\hat{\psi} = \hat{\psi}\hat{\psi}^\dagger$. Then since we are using a representation in which the matrix for S is real and symmetric we have

$$\begin{aligned} m &= \langle\psi|S'|\psi\rangle = \langle\psi|(S \otimes I - I \otimes S)|\psi\rangle \\ &= \mathrm{Tr}(\hat{\psi}\hat{\psi}^\dagger S) - \mathrm{Tr}(\hat{\psi}^\dagger\hat{\psi}S) = 0. \end{aligned}$$

It remains to show the reflection positivity (A2). We may rewrite

$$\begin{aligned} \langle\psi|H'|\psi\rangle = {} & \mathrm{Tr}\,(\hat{\psi}\hat{\psi}^\dagger H_L) + \mathrm{Tr}\,(\hat{\psi}^\dagger\hat{\psi}H_L) \\ & - \tfrac{1}{2}\sum_{\mathbf{x}\in M_L} [\mathrm{Tr}(\hat{\psi}^\dagger S_{\mathbf{x}}^+\hat{\psi}S_{\mathbf{x}}^-) + \mathrm{Tr}(\hat{\psi}^\dagger S_{\mathbf{x}}^-\hat{\psi}S_{\mathbf{x}}^+)]. \end{aligned} \quad \text{(A3)}$$

Here M_L denotes the set of sites in Λ_L that connect to a bond in M, i.e., sites in Λ_L that are nearest neighbor to a site in Λ_R.

We have used that the operators $S_{\mathbf{x}}^\pm$ are represented by real matrices in the standard basis.

The inequality (A2) now follows from the inequality

$$\begin{aligned} \mathrm{Tr}(\hat{\psi}^\dagger A\hat{\psi}A^\dagger) \leq {} & \{\mathrm{Tr}\,[(\hat{\psi}\hat{\psi}^\dagger)^{1/2}A(\hat{\psi}\hat{\psi}^\dagger)^{1/2}A^\dagger]\}^{1/2} \\ & \times \{\mathrm{Tr}\,[(\hat{\psi}^\dagger\hat{\psi})^{1/2}A(\hat{\psi}^\dagger\hat{\psi})^{1/2}A^\dagger]\}^{1/2}, \end{aligned}$$

which holds for any operator A. This inequality is a simple application of the Cauchy-Schwarz inequality if one uses polar decomposition, i.e., the existence of a partial isometry U such that

$$\hat{\psi} = U(\hat{\psi}^\dagger\hat{\psi})^{1/2} \text{ and } (\hat{\psi}\hat{\psi}^\dagger)^{1/2} = U(\hat{\psi}^\dagger\hat{\psi})^{1/2}U^\dagger.$$

At positive temperature we may consider the partition function for H restricted to the subspaces with fixed value of $\Sigma_{\mathbf{x}} S_{\mathbf{x}}^3$. We define

$$Z(m) = \mathrm{Tr}\ \mathcal{P}_m \exp(-\beta H),$$

where $\mathcal{P}_m$ is the projection onto the eigenspace of $\Sigma_{\mathbf{x}} S_{\mathbf{x}}^3$ corresponding to the eigenvalue m. We claim that the partition function is maximal at half filling, i.e.,

$$Z(m) \leq Z(0). \quad \text{(A4)}$$

To prove this we shall again use reflection positivity.

We first note that the unitary change which mapped H to H' will take $\mathcal{P}_m$ into the operator

$$\mathcal{P}'_m = \sum_n P_n \otimes P_{n-m},$$

where P_n is the projection operator in $\mathcal{H}_1$ projecting onto the eigenspace of S with eigenvalue n. Observe that P_m is a real matrix in the standard basis.

Using the Trotter product formula we may now write

$$\begin{aligned} Z(m) = {} & \lim_{k\to\infty} \mathrm{Tr}\ \mathcal{P}'_m \\ & \times \left(e^{-(\beta/k)H_L \otimes I} e^{-(\beta/k) I \otimes H_L} e^{(\beta/2k)\Sigma_M\, S_{\mathbf{x}}^+ S_{\mathbf{y}}^+} e^{(\beta/2k)\Sigma_M\, S_{\mathbf{x}}^- S_{\mathbf{y}}^-}\right)^k. \end{aligned}$$

If we use that

$$e^{(\beta/2k)\Sigma_{\langle\mathbf{xy}\rangle\in M}\, S_{\mathbf{x}}^\pm S_{\mathbf{y}}^\pm} = \prod_{\langle\mathbf{xy}\rangle\in M} \left(1 + \frac{\beta}{2k} S_{\mathbf{x}}^\pm S_{\mathbf{y}}^\pm\right),$$

we see that the trace above may be written as sums of terms of the form $A_n A_{n-m}$, where

$$A_n = \mathrm{Tr}_{\mathcal{H}_1}\,(P_n e^{-\beta H_L/k} T_1 e^{-\beta H_L/k} T_2 \cdots e^{-\beta H_L/k} T_k),$$

and each of the operators $T_1, T_2 \ldots$ is a monomial in the variables $(\beta/2k)^{1/2} S_{\mathbf{x}}^\pm$, $\mathbf{x} \in M_L$.

Since A_n is real for all n we see that $A_n A_{n-m} \leq A_n^2/2 + A_{n-m}^2/2$. If we insert this above and simply undo the calculation we arrive at Eq. (A4).

APPENDIX B: REFLECTION POSITIVITY CONTOUR BOUND

In this appendix we derive Lemma 3, using reflection positivity arguments.

The measures $v_\zeta(d\omega)$ are reflection positive in the following sense. Draw a hyperplane, either vertically (through bonds) or horizontally, that divides $\Gamma=\Lambda\times[0,\beta]$ into two congruent parts $\Gamma_L\cup\Gamma_R$. For any configuration ω, let $\bar{\omega}$ be its natural reflection through the hyperplane (reversing its direction), and for any function h on the space of configurations let $\tilde{h}(\omega)=h(\bar{\omega})$. Then, for any such complex valued function that depends only on the restriction of ω to Γ_L,

$$\int_{\mathcal{A}^\circ} h(\omega)\tilde{h}(\omega)^* e^{-\lambda|\omega|}\, v_\zeta(d\omega) \geq 0. \tag{B1}$$

This can be seen by noting that once the behavior of ω on the hyperplane is fixed, the distribution of the left and right sides (or top and bottom) are conditionally independent, and are mirror images of each other.

Reflection positivity leads to what is known as the *chessboard inequality* [25,26]. In essence, it is a multiply reflected generalization of the Schwarz inequality, which allows us to obtain bounds on the expectation value of a product of local variables in terms of thermodynamic quantities.

The function whose average we need to estimate is $\chi_D(\omega)$—the indicator function which is 1 if the curves in ω avoid a specified set $D\subset\Gamma$ and 0 otherwise. One may start by partitioning the imaginary time interval $[0,\beta]$, and correspondingly the space-time Γ, into equal short segments whose reflections tile Γ. For any subset $D\subset\Gamma$ that is a union of elements of the finite partition of Γ the strategy, which is explained in detail in Ref. [25], yields

$$\frac{\int_{\mathcal{A}^\circ} v_\zeta(d\omega)\chi_D(\omega)e^{-\lambda|\omega|}}{\int_{\mathcal{A}^\circ} v_\zeta(d\omega)e^{-\lambda|\omega|}} \leq \left(\frac{\int_{\mathcal{A}^\circ} v_\zeta(d\omega)\chi_\Gamma(\omega)e^{-\lambda|\omega|}}{\int_{\mathcal{A}^\circ} v_\zeta(d\omega)e^{-\lambda|\omega|}}\right)^{|D|/|\Gamma|} = e^{f|D|}, \tag{B2}$$

where $|D|$ is the total length of D. By refining the partition, and applying elementary continuity arguments (the dominated convergence theorem), we conclude that Eq. (B2) extends to all sets D which are finite unions of closed intervals. This proves Eq. (22).

To prove the second statement in Lemma 3 we note that reflection positivity holds also for the restriction of the measure to ω's with 0 winding number. I.e., for h as in Eq. (B1),

$$\int_{\mathcal{A}^\circ} h(\omega)\tilde{h}(\omega)^*\, I[\nu(\omega)=0]e^{-\lambda|\omega|}\, v_\zeta(d\omega) \geq 0.$$

If the hyperplane dividing Γ into $\Gamma_L\cup\Gamma_R$ is horizontal, this is clear, since fixing ω on this hyperplane fixes the winding number. If it is vertical, however, we note that $I[\nu(\omega)=0]$ can be written as $\Sigma_k I_k(\omega)\tilde{I}_k(\omega)$, where k runs from 0 to $|\Lambda|/2$, and I_k is the indicator function for ω restricted to Γ_L having winding number k. (Note that ω restricted to Γ_L may have sources and sinks on the boundary, and when counting the winding number we also have to consider the curves resulting from these.) The second claim made in Lemma 3 follows by proceeding as in Eq. (B2), but with the added restriction to 0 winding number.

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THE QUANTUM-MECHANICAL MANY-BODY PROBLEM: THE BOSE GAS

ELLIOTT H. LIEB, ROBERT SEIRINGER, JAN PHILIP SOLOVEJ, AND JAKOB YNGVASON

ABSTRACT. Now that the low temperature properties of quantum-mechanical many-body systems (bosons) at low density, ρ, can be examined experimentally it is appropriate to revisit some of the formulas deduced by many authors 4–5 decades ago, and to explore new regimes not treated before. For systems with repulsive (i.e. positive) interaction potentials the experimental low temperature state and the ground state are effectively synonymous – and this fact is used in all modeling. In such cases, the leading term in the energy/particle is $2\pi\hbar^2 a\rho/m$ where a is the scattering length of the two-body potential. Owing to the delicate and peculiar nature of bosonic correlations (such as the strange $N^{7/5}$ law for charged bosons), four decades of research failed to establish this plausible formula rigorously. The only previous lower bound for the energy was found by Dyson in 1957, but it was 14 times too small. The correct asymptotic formula has been obtained by us and this work will be presented. The reason behind the mathematical difficulties will be emphasized. A different formula, postulated as late as 1971 by Schick, holds in two dimensions and this, too, will be shown to be correct. With the aid of the methodology developed to prove the lower bound for the homogeneous gas, several other problems have been successfully addressed. One is the proof by us that the Gross-Pitaevskii equation correctly describes the ground state in the 'traps' actually used in the experiments. For this system it is also possible to prove complete Bose condensation and superfluidity, as we have shown. On the frontier of experimental developments is the possibility that a dilute gas in an elongated trap will behave like a one-dimensional system; we have proved this mathematically. Another topic is a proof that Foldy's 1961 theory of a high density Bose gas of charged particles correctly describes its ground state energy; using this we can also prove the $N^{7/5}$ formula for the ground state energy of the two-component charged Bose gas proposed by Dyson in 1967. All of this is quite recent work and it is hoped that the mathematical methodology might be useful, ultimately, to solve more complex problems connected with these interesting systems.

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FOREWORD

At the conference "Perspectives in Analysis" at the KTH, Stockholm, June 23, 2003, one of us (E.H.L.) contributed a talk with the title above. This talk covered material by all the authors listed above. This contribution is a much expanded version of the talk and of [L4]. It is based on, but supersedes, the article [LSSY].

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1. INTRODUCTION

Schrödinger's equation of 1926 defined a new mechanics whose Hamiltonian is based on classical mechanics, but whose consequences are sometimes non-intuitive from the classical point of view. One of the most extreme cases is the behavior of the ground (= lowest energy) state of a many-body system of particles. Since the ground state function $\Psi(\vec{x}_1, ..., \vec{x}_N)$ is automatically symmetric in the coordinates $\vec{x}_j \in \mathbb{R}^3$ of the N particles, we are dealing

necessarily with *'bosons'*. If we imposed the Pauli exclusion principle (antisymmetry) instead, appropriate for electrons, the outcome would look much more natural and, oddly, more classical. Indeed, the Pauli principle is *essential* for understanding the stability of the ordinary matter that surrounds us.

Recent experiments have confirmed some of the bizarre properties of bosons close to their ground state, but the theoretical ideas go back to the 1940's – 1960's. The first sophisticated analysis of a gas or liquid of *interacting* bosons is due to Bogolubov in 1947. His approximate theory as amplified by others, is supposed to be exact in certain limiting cases, and some of those cases have now been verified rigorously (for the ground state energy) — 3 or 4 decades after they were proposed.

The discussion will center around five main topics.

1. The dilute, homogeneous Bose gas with repulsive interaction (2D and 3D).
2. Repulsive bosons in a trap (as used in recent experiments) and the "Gross-Pitaevskii" equation.
3. Bose condensation and superfluidity for dilute trapped gases.
4. One-dimensional behavior of three-dimensional gases in elongated traps.
5. Foldy's "jellium" model of charged particles in a neutralizing background and the extension to the two-component gas.

Note that for potentials that tend to zero at infinity 'repulsive' and 'positive' are synonymous — in the quantum mechanical literature at least. In classical mechanics, in contrast, a potential that is positive but not monotonically decreasing is not called repulsive.

The discussion below of topic 1 is based on [LY1] and [LY2], and of topic 2 on [LSeY1] and [LSeY2]. See also [LY3, LSeY3, Se2, LSeY4].

The original references for topic 3 are [LSe] and [LSeY5], but for transparency we also include here a section on the special case when the trap is a rectangular box. This case already contains the salient points, but avoids several complications due the inhomogeneity of the gas in a general trap. An essential technical tool for topic 3 is a generalized Poincaré inequality, which is discussed in a separate section.

Topic 4 is a summary of the work in [LSeY6].

The discussion of topic 5 is based on [LSo] and [LSo2].

Topic 1 (3-dimensions) was the starting point and contains essential ideas. It is explained here in some detail and is taken, with minor modifications (and corrections), from [LY3]. In terms of technical complexity, however, the fifth topic is the most involved and can not be treated here in full detail.

The interaction potential between pairs of particles in the Jellium model in topic 5 is the repulsive, *long-range* Coulomb potential, while in topics 1–4 it is assumed to be repulsive and *short range*. For alkali atoms in the recent experiments on Bose Einstein condensation the interaction potential

has a repulsive hard core, but also a quite deep attractive contribution of van der Waals type and there are many two body bound states [PS]. The Bose condensate seen in the experiments is thus not the true ground state (which would be a solid) but a metastable state. Nevertheless, it is usual to model this metastable state as the ground state of a system with a repulsive two body potential having the same scattering length as the true potential, and this is what we shall do. In this paper all interaction potentials will be positive.

2. The Dilute Bose Gas in 3D

We consider the Hamiltonian for N bosons of mass m enclosed in a cubic box Λ of side length L and interacting by a spherically symmetric pair potential $v(|\vec{x}_i - \vec{x}_j|)$:

$$H_N = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} v(|\vec{x}_i - \vec{x}_j|). \tag{2.1}$$

Here $\vec{x}_i \in \mathbb{R}^3$, $i = 1, \dots, N$ are the positions of the particles, Δ_i the Laplacian with respect to $\vec{x}_i$, and we have denoted $\hbar^2/2m$ by μ for short. (By choosing suitable units μ could, of course, be eliminated, but we want to keep track of the dependence of the energy on Planck's constant and the mass.) The Hamiltonian (2.1) operates on *symmetric* wave functions in $L^2(\Lambda^N, d\vec{x}_1 \cdots d\vec{x}_N)$ as is appropriate for bosons. The interaction potential will be assumed to be *nonnegative* and to decrease faster than $1/r^3$ at infinity.

We are interested in the ground state energy $E_0(N, L)$ of (2.1) in the *thermodynamic limit* when N and L tend to infinity with the density $\rho = N/L^3$ fixed. The energy per particle in this limit is

$$e_0(\rho) = \lim_{L \to \infty} E_0(\rho L^3, L)/(\rho L^3). \tag{2.2}$$

Our results about $e_0(\rho)$ are based on estimates on $E_0(N, L)$ for finite N and L, which are important, e.g., for the considerations of inhomogeneous systems in [LSeY1]. To define $E_0(N, L)$ precisely one must specify the boundary conditions. These should not matter for the thermodynamic limit. To be on the safe side we use Neumann boundary conditions for the lower bound, and Dirichlet boundary conditions for the upper bound since these lead, respectively, to the lowest and the highest energies.

For experiments with dilute gases the *low density asymptotics* of $e_0(\rho)$ is of importance. Low density means here that the mean interparticle distance, $\rho^{-1/3}$ is much larger than the *scattering length* a of the potential, which is defined as follows. The zero energy scattering Schrödinger equation

$$-2\mu\Delta\psi + v(r)\psi = 0 \tag{2.3}$$

has a solution of the form, asymptotically as $|\vec{x}| = r \to \infty$ (or for all $r > R_0$ if $v(r) = 0$ for $r > R_0$),

$$\psi_0(\vec{x}) = 1 - a/|\vec{x}| \tag{2.4}$$

(The factor 2 in (2.3) comes from the reduced mass of the two particle problem.) Writing $\psi_0(\vec{x}) = u_0(|\vec{x}|)/|\vec{x}|$ this is the same as

$$a = \lim_{r\to\infty} r - \frac{u_0(r)}{u_0'(r)}, \tag{2.5}$$

where u_0 solves the zero energy (radial) scattering equation,

$$-2\mu u_0''(r) + v(r)u_0(r) = 0 \tag{2.6}$$

with $u_0(0) = 0$.

An important special case is the hard core potential $v(r) = \infty$ if $r < a$ and $v(r) = 0$ otherwise. Then the scattering length a and the radius a are the same.

Our main result is a rigorous proof of the formula

$$e_0(\rho) \approx 4\pi\mu\rho a \tag{2.7}$$

for $\rho a^3 \ll 1$, more precisely of

Theorem 2.1 (Low density limit of the ground state energy).

$$\lim_{\rho a^3\to 0} \frac{e_0(\rho)}{4\pi\mu\rho a} = 1. \tag{2.8}$$

This formula is independent of the boundary conditions used for the definition of $e_0(\rho)$. It holds for every positive radially symmetric pair potential such that $\int_R^\infty v(r)r^2dr < \infty$ for some R, which guarantees a finite scattering length, cf. Appendix A in [LY2].

The genesis of an understanding of $e_0(\rho)$ was the pioneering work [Bo] of Bogolubov, and in the 50's and early 60's several derivations of (2.8) were presented [HY], [L1], even including higher order terms:

$$\frac{e_0(\rho)}{4\pi\mu\rho a} = 1 + \tfrac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\left(\tfrac{4\pi}{3} - \sqrt{3}\right)(\rho a^3)\log(\rho a^3) + O(\rho a^3) \tag{2.9}$$

These early developments are reviewed in [L2]. They all rely on some special assumptions about the ground state that have never been proved, or on the selection of special terms from a perturbation series which likely diverges. The only rigorous estimates of this period were established by Dyson, who derived the following bounds in 1957 for a gas of hard spheres [D1]:

$$\frac{1}{10\sqrt{2}} \le \frac{e_0(\rho)}{4\pi\mu\rho a} \le \frac{1 + 2Y^{1/3}}{(1 - Y^{1/3})^2} \tag{2.10}$$

with $Y = 4\pi\rho a^3/3$. While the upper bound has the asymptotically correct form, the lower bound is off the mark by a factor of about 1/14. But for about 40 years this was the best lower bound available!

Under the assumption that (2.8) is a correct asymptotic formula for the energy, we see at once that understanding it physically, much less proving it,

is not a simple matter. Initially, the problem presents us with two lengths, $a \ll \rho^{-1/3}$ at low density. However, (2.8) presents us with another length generated by the solution to the problem. This length is the de Broglie wavelength, or 'uncertainty principle' length (sometimes called 'healing length')

$$\ell_c \sim (\rho a)^{-1/2}. \tag{2.11}$$

The reason for saying that ℓ_c is the de Broglie wavelength is that in the hard core case all the energy is kinetic (the hard core just imposes a $\psi = 0$ boundary condition whenever the distance between two particles is less than a). By the uncertainty principle, the kinetic energy is proportional to an inverse length squared, namely ℓ_c. We then have the relation (since ρa^3 is small)

$$a \ll \rho^{-1/3} \ll \ell_c \tag{2.12}$$

which implies, physically, that it is impossible to localize the particles relative to each other (even though ρ is small). Bosons in their ground state are therefore 'smeared out' over distances large compared to the mean particle distance and their individuality is entirely lost. They cannot be localized with respect to each other without changing the kinetic energy enormously.

Fermions, on the other hand, prefer to sit in 'private rooms', i.e., ℓ_c is never bigger than $\rho^{-1/3}$ by a fixed factor. In this respect the quantum nature of bosons is much more pronounced than for fermions.

Since (2.8) is a basic result about the Bose gas it is clearly important to derive it rigorously and in reasonable generality, in particular for more general cases than hard spheres. The question immediately arises for which interaction potentials one may expect it to be true. A notable fact is that it *is not true for all* v with $a > 0$, since there are two body potentials with positive scattering length that allow many body bound states. (There are even such potentials without two body bound states but with three body bound states [Ba].) For such potentials (2.8) is clearly false. Our proof, presented in the sequel, works for nonnegative v, but we conjecture that (2.8) holds if $a > 0$ and v has no N-body bound states for any N. The lower bound is, of course, the hardest part, but the upper bound is not altogether trivial either.

Before we start with the estimates a simple computation and some heuristics may be helpful to make (2.8) plausible and motivate the formal proofs.

With ψ_0 the zero energy scattering solution, partial integration, using (2.3) and (2.4), gives, for $R \geq R_0$,

$$\int_{|\vec{x}|\leq R} \{2\mu|\nabla\psi_0|^2 + v|\psi_0|^2\} d\vec{x} = 8\pi\mu a \left(1 - \frac{a}{R}\right) \to 8\pi\mu a \quad \text{for } R \to \infty. \tag{2.13}$$

Moreover, for positive interaction potentials the scattering solution minimizes the quadratic form in (2.13) for each $R \geq R_0$ with the boundary condition $\psi_0(|\vec{x}| = R) = (1 - a/R)$. Hence the energy $E_0(2, L)$ of two particles

in a large box, i.e., $L \gg a$, is approximately $8\pi\mu a/L^3$. If the gas is sufficiently dilute it is not unreasonable to expect that the energy is essentially a sum of all such two particle contributions. Since there are $N(N-1)/2$ pairs, we are thus lead to $E_0(N,L) \approx 4\pi\mu a N(N-1)/L^3$, which gives (2.8) in the thermodynamic limit.

This simple heuristics is far from a rigorous proof, however, especially for the lower bound. In fact, it is rather remarkable that the same asymptotic formula holds both for 'soft' interaction potentials, where perturbation theory can be expected to be a good approximation, and potentials like hard spheres where this is not so. In the former case the ground state is approximately the constant function and the energy is *mostly potential*: According to perturbation theory $E_0(N,L) \approx N(N-1)/(2L^3)\int v(|\vec{x}|)d\vec{x}$. In particular it is *independent of* μ, i.e. of Planck's constant and mass. Since, however, $\int v(|\vec{x}|)d\vec{x}$ is the first Born approximation to $8\pi\mu a$ (note that a depends on μ!), this is not in conflict with (2.8). For 'hard' potentials on the other hand, the ground state is *highly correlated*, i.e., it is far from being a product of single particle states. The energy is here *mostly kinetic*, because the wave function is very small where the potential is large. These two quite different regimes, the potential energy dominated one and the kinetic energy dominated one, cannot be distinguished by the low density asymptotics of the energy. Whether they behave differently with respect to other phenomena, e.g., Bose-Einstein condensation, is not known at present.

Bogolubov's analysis [Bo] presupposes the existence of Bose-Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [LL], despite the fact that there is (presumably) no condensation in that case [PiSt]. It turns out that BE condensation is not really needed in order to understand the energy. As we shall see, 'global' condensation can be replaced by a 'local' condensation on boxes whose size is independent of L. It is this crucial understanding that enables us to prove Theorem 1.1 without having to decide about BE condensation.

An important idea of Dyson was to transform the hard sphere potential into a soft potential at the cost of sacrificing the kinetic energy, i.e., effectively to move from one regime to the other. We shall make use of this idea in our proof of the lower bound below. But first we discuss the simpler upper bound, which relies on other ideas from Dyson's beautiful paper [D1].

2.1. **Upper Bound.** The following generalization of Dyson's upper bound holds [LSeY1], [Se1]:

Theorem 2.2 (Upper bound). *Let* $\rho_1 = (N-1)/L^3$ *and* $b = (4\pi\rho_1/3)^{-1/3}$. *For non-negative potentials* v *and* $b > a$ *the ground state energy of (2.1) with periodic boundary conditions satisfies*

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \frac{a}{b} + \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1 - \frac{a}{b}\right)^8}. \tag{2.14}$$

Thus in the thermodynamic limit (and for all boundary conditions)

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1 - Y^{1/3} + Y^{2/3} - \frac{1}{2}Y}{(1 - Y^{1/3})^8}, \tag{2.15}$$

provided $Y = 4\pi\rho a^3/3 < 1$.

Remark. The bound (2.14) holds for potentials with infinite range, provided $b > a$. For potentials of finite range R_0 it can be improved for $b > R_0$ to

$$E_0(N, L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1 - \frac{a}{b}\right)^4}. \tag{2.16}$$

Proof. We first remark that the expectation value of (2.1) with any trial wave function gives an upper bound to the bosonic ground state energy, even if the trial function is not symmetric under permutations of the variables. The reason is that an absolute ground state of the elliptic differential operator (2.1) (i.e., a ground state without symmetry requirement) is a nonnegative function which can be symmetrized without changing the energy because (2.1) is symmetric under permutations. In other words, the absolute ground state energy is the same as the bosonic ground state energy.

Following [D1] we choose a trial function of the following form

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = F_1(\vec{x}_1) \cdot F_2(\vec{x}_1, \vec{x}_2) \cdots F_N(\vec{x}_1, \ldots, \vec{x}_N). \tag{2.17}$$

More specifically, $F_1 \equiv 1$ and F_i depends only on the distance of $\vec{x}_i$ to its nearest neighbor among the points $\vec{x}_1, \ldots, \vec{x}_{i-1}$ (taking the periodic boundary into account):

$$F_i(\vec{x}_1, \ldots, \vec{x}_i) = f(t_i), \quad t_i = \min\left(|\vec{x}_i - \vec{x}_j|, j = 1, \ldots, i-1\right), \tag{2.18}$$

with a function f satisfying

$$0 \leq f \leq 1, \quad f' \geq 0. \tag{2.19}$$

The intuition behind the ansatz (2.17) is that the particles are inserted into the system one at the time, taking into account the particles previously inserted. While such a wave function cannot reproduce all correlations present in the true ground state, it turns out to capture the leading term in the energy for dilute gases. The form (2.17) is computationally easier to handle than an ansatz of the type $\prod_{i<j} f(|\vec{x}_i - \vec{x}_j|)$, which might appear more natural in view of the heuristic remarks after Eq. (2.13).

The function f is chosen to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \leq r \leq b, \\ 1 & \text{for } r > b, \end{cases} \tag{2.20}$$

with $f_0(r) = u_0(r)/r$ the zero energy scattering solution defined by (2.6). The estimates (2.14) and (2.16) are obtained by somewhat lengthy computations similar as in [D1], but making use of (2.13). For details we refer to [LSeY1] and [Se1]. ∎

2.2. **Lower Bound.** It was explained previously in this section why the lower bound for the bosonic ground state energy of (2.1) is not easy to obtain. The three different length scales (2.12) for bosons will play a role in the proof below.

- The scattering length a.
- The mean particle distance $\rho^{-1/3}$.
- The 'uncertainty principle length' ℓ_c, defined by $\mu\ell_c^{-2} = e_0(\rho)$, i.e., $\ell_c \sim (\rho a)^{-1/2}$.

Our lower bound for $e_0(\rho)$ is as follows.

Theorem 2.3 (Lower bound in the thermodynamic limit). *For a positive potential v with finite range and Y small enough*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \geq (1 - CY^{1/17}) \tag{2.21}$$

with C a constant. If v does not have finite range, but decreases faster than $1/r^3$ (more precisely, $\int_R^\infty v(r)r^2dr < \infty$ for some R) then an analogous bound to (2.21) holds, but with $CY^{1/17}$ replaced by $o(1)$ as $Y \to 0$.

It should be noted right away that the error term $-CY^{1/17}$ in (2.21) is of no fundamental significance and is not believed to reflect the true state of affairs. Presumably, it does not even have the right sign. We mention in passing that C can be taken to be 8.9 [Se1].

As mentioned at the beginning of this section after Eq. (2.2), a lower bound on $E_0(N, L)$ for finite N and L is of importance for applications to inhomogeneous gases, and in fact we derive (2.21) from such a bound. We state it in the following way:

Theorem 2.4 (Lower bound in a finite box). *For a positive potential v with finite range there is a $\delta > 0$ such that the ground state energy of (2.1) with Neumann boundary conditions satisfies*

$$E_0(N, L)/N \geq 4\pi\mu\rho a\left(1 - CY^{1/17}\right) \tag{2.22}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are positive constants, independent of N and L. (Note that the condition on L/a requires in particular that N must be large enough, $N >$ (const.)$Y^{-1/17}$.) As in Theorem 2.3 such a bound, but possibly with a different error term holds also for potentials v of infinite range that decrease sufficiently fast at infinity.

The first step in the proof of Theorem 2.4 is a generalization of a lemma of Dyson, which allows us to replace v by a 'soft' potential, at the cost of sacrificing kinetic energy and increasing the effective range.

Lemma 2.5. *Let $v(r) \geq 0$ with finite range R_0. Let $U(r) \geq 0$ be any function satisfying $\int U(r)r^2dr \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $\mathcal{B} \subset \mathbb{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all*

differentiable functions ψ

$$\int_{\mathcal{B}} [\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2] \geq \mu a \int_{\mathcal{B}} U|\psi|^2. \tag{2.23}$$

Proof. Actually, (2.23) holds with $\mu|\nabla\psi(\vec{x})|^2$ replaced by the (smaller) radial kinetic energy, $\mu|\partial\psi(\vec{x})/\partial r|^2$, and it suffices to prove the analog of (2.23) for the integral along each radial line with fixed angular variables. Along such a line we write $\psi(\vec{x}) = u(r)/r$ with $u(0) = 0$. We consider first the special case when U is a delta-function at some radius $R \geq R_0$, i.e.,

$$U(r) = \frac{1}{R^2}\delta(r - R). \tag{2.24}$$

For such U the analog of (2.23) along the radial line is

$$\int_0^{R_1} \{\mu[u'(r) - (u(r)/r)]^2 + \tfrac{1}{2}v(r)|u(r)]^2\}dr \geq \begin{cases} 0 & \text{if } R_1 < R \\ \mu a|u(R)|^2/R^2 & \text{if } R \leq R_1 \end{cases} \tag{2.25}$$

where R_1 is the length of the radial line segment in $\mathcal{B}$. The case $R_1 < R$ is trivial, because $\mu|\partial\psi/\partial r|^2 + \frac{1}{2}v|\psi|^2 \geq 0$. (Note that positivity of v is used here.) If $R \leq R_1$ we consider the integral on the left side of (2.25) from 0 to R instead of R_1 and minimize it under the boundary condition that $u(0) = 0$ and $u(R)$ is a fixed constant. Since everything is homogeneous in u we may normalize this value to $u(R) = R - a$. This minimization problem leads to the zero energy scattering equation (2.6). Since v is positive, the solution is a true minimum and not just a stationary point.

Because $v(r) = 0$ for $r > R_0$ the solution, u_0, satisfies $u_0(r) = r - a$ for $r > R_0$. By partial integration,

$$\int_0^R \{\mu[u_0'(r) - (u_0(r)/r)]^2 + \tfrac{1}{2}v(r)|u_0(r)]^2\}dr = \mu a|R-a|/R \geq \mu a|R-a|^2/R^2. \tag{2.26}$$

But $|R-a|^2/R^2$ is precisely the right side of (2.25) if u satisfies the normalization condition.

This derivation of (2.23) for the special case (2.24) implies the general case, because every U can be written as a superposition of δ-functions, $U(r) = \int R^{-2}\delta(r-R)\,U(R)R^2dR$, and $\int U(R)R^2dR \leq 1$ by assumption. ■

By dividing Λ for given points $\vec{x}_1, \ldots, \vec{x}_N$ into Voronoi cells $\mathcal{B}_i$ that contain all points closer to $\vec{x}_i$ than to $\vec{x}_j$ with $j \neq i$ (these cells are star shaped w.r.t. $\vec{x}_i$, indeed convex), the following corollary of Lemma 2.5 can be derived in the same way as the corresponding Eq. (28) in [D1].

Corollary 2.6. *For any U as in Lemma 2.5*

$$H_N \geq \mu a W \tag{2.27}$$

with W the multiplication operator

$$W(\vec{x}_1, \ldots, \vec{x}_N) = \sum_{i=1}^{N} U(t_i), \tag{2.28}$$

where t_i is the distance of $\vec{x}_i$ to its nearest neighbor among the other points $\vec{x}_j$, $j = 1, \ldots, N$, i.e.,

$$t_i(\vec{x}_1, \ldots, \vec{x}_N) = \min_{j, j \neq i} |\vec{x}_i - \vec{x}_j|. \tag{2.29}$$

(Note that t_i has here a slightly different meaning than in (2.18), where it denoted the distance to the nearest neighbor among the $\vec{x}_j$ with $j \leq i - 1$.)

Dyson considers in [D1] a one parameter family of U's that is essentially the same as the following choice, which is convenient for the present purpose:

$$U_R(r) = \begin{cases} 3(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise.} \end{cases} \tag{2.30}$$

We denote the corresponding interaction (2.28) by W_R. For the hard core gas one obtains

$$E(N, L) \geq \sup_R \inf_{(\vec{x}_1, \ldots, \vec{x}_N)} \mu a W_R(\vec{x}_1, \ldots, \vec{x}_N) \tag{2.31}$$

where the infimum is over $(\vec{x}_1, \ldots, x_N) \in \Lambda^N$ with $|\vec{x}_i - \vec{x}_j| \geq R_0 = a$, because of the hard core. At fixed R simple geometry gives

$$\inf_{(\vec{x}_1, \ldots, \vec{x}_N)} W_R(\vec{x}_1, \ldots, \vec{x}_N) \geq \left(\frac{A}{R^3} - \frac{B}{\rho R^6} \right) \tag{2.32}$$

with certain constants A and B. An evaluation of these constants gives Dyson's bound

$$E(N, L)/N \geq \frac{1}{10\sqrt{2}} 4\pi\mu\rho a. \tag{2.33}$$

The main reason this method does not give a better bound is that R must be chosen quite big, namely of the order of the mean particle distance $\rho^{-1/3}$, in order to guarantee that the spheres of radius R around the N points overlap. Otherwise the infimum of W_R will be zero. But large R means that W_R is small. It should also be noted that this method does not work for potentials other than hard spheres: If $|\vec{x}_i - \vec{x}_j|$ is allowed to be less than R_0, then the right side of (2.31) is zero because $U(r) = 0$ for $r < R_0$.

For these reasons we take another route. We still use Lemma 2.5 to get into the soft potential regime, but we do *not* sacrifice *all* the kinetic energy as in (2.27). Instead we write, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1 - \varepsilon) H_N \geq \varepsilon T_N + (1 - \varepsilon) H_N \tag{2.34}$$

with $T_N = -\sum_i \Delta_i$ and use (2.27) only for the part $(1 - \varepsilon) H_N$. This gives

$$H_N \geq \varepsilon T_N + (1 - \varepsilon) \mu a W_R. \tag{2.35}$$

We consider the operator on the right side from the viewpoint of first order perturbation theory, with εT_N as the unperturbed part, denoted H_0.

The ground state of H_0 in a box of side length L is $\Psi_0(\vec{x}_1,\dots,\vec{x}_N) \equiv L^{-3N/2}$ and we denote expectation values in this state by $\langle\cdot\rangle_0$. A computation, cf. Eq. (21) in [LY1] (see also Eqs. (3.15)–(3.20)), gives

$$\begin{aligned} 4\pi\rho\left(1-\tfrac{1}{N}\right) &\geq \langle W_R\rangle_0/N \\ &\geq 4\pi\rho\left(1-\tfrac{1}{N}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+4\pi\rho(R^3-R_0^3)/3\right)^{-1}. \end{aligned} \tag{2.36}$$

The rationale behind the various factors is as follows: $(1-\frac{1}{N})$ comes from the fact that the number of pairs is $N(N-1)/2$ and not $N^2/2$, $(1-2R/L)^3$ takes into account the fact that the particles do not interact beyond the boundary of Λ, and the last factor measures the probability to find another particle within the interaction range of the potential U_R for a given particle.

The estimates (2.36) on the first order term look at first sight quite promising, for if we let $L\to\infty$, $N\to\infty$ with $\rho = N/L^3$ fixed, and subsequently take $R\to 0$, then $\langle W_R\rangle_0/N$ converges to $4\pi\rho$, which is just what is desired. But the first order result (2.36) is not a rigorous bound on $E_0(N,L)$, we need *error estimates*, and these will depend on ε, R and L.

We now recall *Temple's inequality* [T] for the expectation values of an operator $H = H_0+V$ in the ground state $\langle\cdot\rangle_0$ of H_0. It is a simple consequence of the operator inequality

$$(H-E_0)(H-E_1)\geq 0 \tag{2.37}$$

for the two lowest eigenvalues, $E_0 < E_1$, of H and reads

$$E_0 \geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0} \tag{2.38}$$

provided $E_1 - \langle H\rangle_0 > 0$. Furthermore, if $V\geq 0$ we may use $E_1 \geq E_1^{(0)}=$ second lowest eigenvalue of H_0 and replace E_1 in (2.38) by $E_1^{(0)}$.

From (2.36) and (2.38) we get the estimate

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\left(1-\mathcal{E}(\rho,L,R,\varepsilon)\right) \tag{2.39}$$

with

$$\begin{aligned} &1-\mathcal{E}(\rho,L,R,\varepsilon) \\ &= (1-\varepsilon)\left(1-\tfrac{1}{\rho L^3}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+\tfrac{4\pi}{3}\rho(R^3-R_0^3)\right)^{-1} \\ &\quad\times\left(1-\frac{\mu a\left(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2\right)}{\langle W_R\rangle_0\left(E_1^{(0)} - \mu a\langle W_R\rangle_0\right)}\right). \end{aligned} \tag{2.40}$$

To evaluate this further one may use the estimates (2.36) and the bound

$$\langle W_R^2\rangle_0 \leq 3\frac{N}{R^3-R_0^3}\langle W_R\rangle_0 \tag{2.41}$$

which follows from $U_R^2 = 3(R^3-R_0^3)^{-1}U_R$ together with the Schwarz inequality. A glance at the form of the error term reveals, however, that it

is *not* possible here to take the thermodynamic limit $L \to \infty$ with ρ fixed: We have $E_1^{(0)} = \varepsilon\pi^2\mu/L^2$ (this is the kinetic energy of a *single* particle in the first excited state in the box), and the factor $E_1^{(0)} - \mu a\langle W_R\rangle_0$ in the denominator in (2.40) is, up to unimportant constants and lower order terms, $\sim (\varepsilon L^{-2} - a\rho^2 L^3)$. Hence the denominator eventually becomes negative and Temple's inequality looses its validity if L is large enough.

As a way out of this dilemma we divide the big box Λ into cubic *cells* of side length ℓ that is kept *fixed* as $L \to \infty$. The number of cells, L^3/ℓ^3, on the other hand, increases with L. The N particles are distributed among these cells, and we use (2.40), with L replaced by ℓ, N by the particle number, n, in a cell and ρ by n/ℓ^3, to estimate the energy in each cell with *Neumann* conditions on the boundary. For each distribution of the particles we add the contributions from the cells, neglecting interactions across boundaries. Since $v \geq 0$ by assumption, this can only lower the energy. Finally, we minimize over all possible choices of the particle numbers for the various cells adding up to N. The energy obtained in this way is a lower bound to $E_0(N, L)$, because we are effectively allowing discontinuous test functions for the quadratic form given by H_N.

In mathematical terms, the cell method leads to

$$E_0(N, L)/N \geq (\rho\ell^3)^{-1} \inf \sum_{n\geq 0} c_n E_0(n, \ell) \tag{2.42}$$

where the infimum is over all choices of coefficients $c_n \geq 0$ (relative number of cells containing exactly n particles), satisfying the constraints

$$\sum_{n\geq 0} c_n = 1, \qquad \sum_{n\geq 0} c_n n = \rho\ell^3. \tag{2.43}$$

The minimization problem for the distributions of the particles among the cells would be easy if we knew that the ground state energy $E_0(n, \ell)$ (or a good lower bound to it) were convex in n. Then we could immediately conclude that it is best to have the particles as evenly distributed among the boxes as possible, i.e., c_n would be zero except for the n equal to the integer closest to $\rho\ell^3$. This would give

$$\frac{E_0(N, L)}{N} \geq 4\pi\mu a\rho\,(1 - \mathcal{E}(\rho, \ell, R, \varepsilon)) \tag{2.44}$$

i.e., replacement of L in (2.39) by ℓ, which is independent of L. The blow up of $\mathcal{E}$ for $L \to \infty$ would thus be avoided.

Since convexity of $E_0(n, \ell)$ is not known (except in the thermodynamic limit) we must resort to other means to show that $n = O(\rho\ell^3)$ in all boxes. The rescue comes from *superadditivity* of $E_0(n, \ell)$, i.e., the property

$$E_0(n + n', \ell) \geq E_0(n, \ell) + E_0(n', \ell) \tag{2.45}$$

which follows immediately from $v \geq 0$ by dropping the interactions between the n particles and the n' particles. The bound (2.45) implies in particular

that for any $n, p \in \mathbb{N}$ with $n \geq p$

$$E_0(n,\ell) \geq [n/p]\, E_0(p,\ell) \geq \frac{n}{2p} E_0(p,\ell) \tag{2.46}$$

since the largest integer $[n/p]$ smaller than n/p is in any case $\geq n/(2p)$.

The way (2.46) is used is as follows: Replacing L by ℓ, N by n and ρ by n/ℓ^3 in (2.39) we have for fixed R and ε

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(n,\ell) \tag{2.47}$$

with a certain function $K(n,\ell)$ determined by (2.40). We shall see that K is monotonously decreasing in n, so that if $p \in \mathbb{N}$ and $n \leq p$ then

$$E_0(n,\ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(p,\ell). \tag{2.48}$$

We now split the sum in (2.42) into two parts. For $n < p$ we use (2.48), and for $n \geq p$ we use (2.46) together with (2.48) for $n = p$. The task is thus to minimize

$$\sum_{n<p} c_n n(n-1) + \tfrac{1}{2} \sum_{n \geq p} c_n n(p-1) \tag{2.49}$$

subject to the constraints (2.43). Putting

$$k := \rho\ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \leq k \tag{2.50}$$

we have $\sum_{n\geq p} c_n n = k - t$, and since $n(n-1)$ is convex in n and vanishes for $n = 0$, and $\sum_{n<p} c_n \leq 1$, the expression (2.49) is

$$\geq t(t-1) + \tfrac{1}{2}(k-t)(p-1). \tag{2.51}$$

We have to minimize this for $1 \leq t \leq k$. If $p \geq 4k$ the minimum is taken at $t = k$ and is equal to $k(k-1)$. Altogether we have thus shown that

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho \left(1 - \frac{1}{\rho\ell^3}\right) K(4\rho\ell^3, \ell). \tag{2.52}$$

What remains is to take a closer look at $K(4\rho\ell^3,\ell)$, which depends on the parameters ε and R besides ℓ, and choose the parameters in an optimal way. From (2.40) and (2.41) we obtain

$$\begin{aligned} K(n,\ell) &= (1-\varepsilon)\left(1 - \tfrac{2R}{\ell}\right)^3 \left(1 + \tfrac{4\pi}{3}(R^3 - R_0^3)\right)^{-1} \\ &\times \left(1 - \frac{3}{\pi}\frac{an}{(R^3 - R_0^3)(\pi\varepsilon\ell^{-2} - 4a\ell^{-3}n(n-1))}\right). \end{aligned} \tag{2.53}$$

The estimate (2.47) with this K is valid as long as the denominator in the last factor in (2.53) is ≥ 0, and in order to have a formula for all n we can take 0 as a trivial lower bound in other cases or when (2.47) is negative.

As required for (2.48), K is monotonously decreasing in n. We now insert $n = 4\rho\ell^3$ and obtain

$$K(4\rho\ell^3, \ell) \geq (1-\varepsilon)\left(1-\tfrac{2R}{\ell}\right)^3 \left(1+(\text{const.})Y(\ell/a)^3(R^3-R_0^3)/\ell^3\right)^{-1} \times \left(1-\frac{\ell^3}{(R^3-R_0^3)}\frac{(\text{const.})Y}{(\varepsilon(a/\ell)^2-(\text{const.})Y^2(\ell/a)^3)}\right) \tag{2.54}$$

with $Y = 4\pi\rho a^3/3$ as before. Also, the factor

$$\left(1-\frac{1}{\rho\ell^3}\right) = (1-(\text{const.})Y^{-1}(a/\ell)^3) \tag{2.55}$$

in (2.52) (which is the ratio between $n(n-1)$ and n^2) must not be forgotten. We now make the ansatz

$$\varepsilon \sim Y^\alpha, \quad a/\ell \sim Y^\beta, \quad (R^3-R_0^3)/\ell^3 \sim Y^\gamma \tag{2.56}$$

with exponents α, β and γ that we choose in an optimal way. The conditions to be met are as follows:

- $\varepsilon(a/\ell)^2 - (\text{const.})Y^2(\ell/a)^3 > 0$. This holds for all small enough Y, provided $\alpha + 5\beta < 2$ which follows from the conditions below.
- $\alpha > 0$ in order that $\varepsilon \to 0$ for $Y \to 0$.
- $3\beta - 1 > 0$ in order that $Y^{-1}(a/\ell)^3 \to 0$ for for $Y \to 0$.
- $1 - 3\beta + \gamma > 0$ in order that $Y(\ell/a)^3(R^3-R_0^3)/\ell^3 \to 0$ for for $Y \to 0$.
- $1 - \alpha - 2\beta - \gamma > 0$ to control the last factor in (2.54).

Taking

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \tag{2.57}$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - 3\beta + \gamma = 1 - \alpha - 2\beta - \gamma = 1/17. \tag{2.58}$$

It is also clear that $2R/\ell \sim Y^{\gamma/3} = Y^{1/17}$, up to higher order terms. This completes the proof of Theorems 2.3 and 2.4, for the case of potentials with finite range. By optimizing the proportionality constants in (2.56) one can show that $C = 8.9$ is possible in Theorem 2.3 [Se1]. The extension to potentials of infinite range but finite scattering length is obtained by approximation by finite range potentials, controlling the change of the scattering length as the cut-off is removed. See Appendix A in [LY2] and Appendix B in [LSeY1] for details. We remark that a slower decrease of the potential than $1/r^3$ implies infinite scattering length. ■

The exponents (2.57) mean in particular that

$$a \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho a)^{-1/2}, \tag{2.59}$$

whereas Dyson's method required $R \sim \rho^{-1/3}$ as already explained. The condition $\rho^{-1/3} \ll \ell$ is required in order to have many particles in each box and thus $n(n-1) \approx n^2$. The condition $\ell \ll (\rho a)^{-1/2}$ is necessary for a spectral gap $\gg e_0(\rho)$ in Temple's inequality. It is also clear that this choice of ℓ would lead to a far too big energy and no bound for $e_0(\rho)$ if we had

chosen Dirichlet instead of Neumann boundary conditions for the cells. But with the latter the method works!

3. The Dilute Bose Gas in 2D

In contrast to the three-dimensional theory, the two-dimensional Bose gas began to receive attention only relatively late. The first derivation of the correct asymptotic formula was, to our knowledge, done by Schick [S] for a gas of hard discs. He found

$$e(\rho) \approx 4\pi\mu\rho|\ln(\rho a^2)|^{-1}. \tag{3.1}$$

This was accomplished by an infinite summation of 'perturbation series' diagrams. Subsequently, a corrected modification of [S] was given in [HFM]. Positive temperature extensions were given in [Po] and in [FH]. All this work involved an analysis in momentum space, with the exception of a method due to one of us that works directly in configuration space [L1]. Ovchinnikov [O] derived (3.1) by using, basically, the method in [L1]. These derivations require several unproven assumptions and are not rigorous.

In two dimensions the scattering length a is defined using the zero energy scattering equation (2.3) but instead of $\psi(r) \approx 1 - a/r$ we now impose the asymptotic condition $\psi(r) \approx \ln(r/a)$. This is explained in the appendix to [LY2].

Note that in two dimensions the ground state energy could not possibly be $e_0(\rho) \approx 4\pi\mu\rho a$ as in three dimensions because that would be dimensionally wrong. Since $e_0(\rho)$ should essentially be proportional to ρ, there is apparently no room for an a dependence — which is ridiculous! It turns out that this dependence comes about in the $\ln(\rho a^2)$ factor.

One of the intriguing facts about (3.1) is that the energy for N particles is *not equal* to $N(N-1)/2$ times the energy for two particles in the low density limit — as is the case in three dimensions. The latter quantity, $E_0(2, L)$, is, asymptotically for large L, equal to $8\pi\mu L^{-2}\left[\ln(L^2/a^2)\right]^{-1}$. (This is seen in an analogous way as (2.13). The three-dimensional boundary condition $\psi_0(|\vec{x}| = R) = 1 - a/R$ is replaced by $\psi_0(|\vec{x}| = R) = \ln(R/a)$ and moreover it has to be taken into account that with this normalization $\|\psi_0\|^2 = (\text{volume})(\ln(R/a))^2$ (to leading order), instead of just the volume in the three-dimensional case.) Thus, if the $N(N-1)/2$ rule were to apply, (3.1) would have to be replaced by the much smaller quantity $4\pi\mu\rho\left[\ln(L^2/a^2)\right]^{-1}$. In other words, L, which tends to ∞ in the thermodynamic limit, has to be replaced by the mean particle separation, $\rho^{-1/2}$ in the logarithmic factor. Various poetic formulations of this curious fact have been given, but the fact remains that the non-linearity is something that does not occur in more than two dimensions and its precise nature is hardly obvious, physically. This anomaly is the main reason that the two-dimensional case is not a trivial extension of the three-dimensional one.

Eq. (3.1) was proved in [LY2] for nonnegative, finite range two-body potentials by finding upper and lower bounds of the correct form, using similar ideas as in the previous section for the three-dimensional case. We discuss below the modifications that have to be made in the present two-dimensional case. The restriction to finite range can be relaxed as in three dimensions, but the restriction to nonnegative v cannot be removed in the current state of our methodology. The upper bounds will have relative remainder terms $O(|\ln(\rho a^2)|^{-1})$ while the lower bound will have remainder $O(|\ln(\rho a^2)|^{-1/5})$. It is claimed in [HFM] that the relative error for a hard core gas is negative and $O(\ln|\ln(\rho a^2)||\ln(\rho a^2)|^{-1})$, which is consistent with our bounds.

The upper bound is derived in complete analogy with the three dimensional case. The function f_0 in the variational ansatz (2.20) is in two dimensions also the zero energy scattering solution — but for 2D, of course. The result is

$$E_0(N,L)/N \leq \frac{2\pi\mu\rho}{\ln(b/a) - \pi\rho b^2}\left(1 + O([\ln(b/a)]^{-1})\right). \tag{3.2}$$

The minimum over b of the leading term is obtained for $b = (2\pi\rho)^{-1/2}$. Inserting this in (3.2) we thus obtain

$$E_0(N,L)/N \leq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 + O(|\ln(\rho a^2)|^{-1})\right). \tag{3.3}$$

To prove the lower bound the essential new step is to modify Dyson's lemma for 2D. The 2D version of Lemma 2.5 is:

Lemma 3.1. *Let $v(r) \geq 0$ and $v(r) = 0$ for $r > R_0$. Let $U(r) \geq 0$ be any function satisfying*

$$\int_0^\infty U(r)\ln(r/a)rdr \leq 1 \text{ and } U(r) = 0 \text{ for } r < R_0. \tag{3.4}$$

Let $\mathcal{B} \subset \mathbb{R}^2$ be star-shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then, for all functions ψ in the Sobolev space $H^1(\mathcal{B})$,

$$\int_{\mathcal{B}} \left(\mu|\nabla\psi(\vec{x})|^2 + \tfrac{1}{2}v(|\vec{x}|)|\psi(\vec{x})|^2\right) d\vec{x} \geq \mu\int_{\mathcal{B}} U(|\vec{x}|)|\psi(\vec{x})|^2\, d\vec{x}. \tag{3.5}$$

Proof. In polar coordinates, r,θ, one has $|\nabla\psi|^2 \geq |\partial\psi/\partial r|^2$. Therefore, it suffices to prove that for each angle $\theta \in [0,2\pi)$, and with $\psi(r,\theta)$ denoted simply by $f(r)$,

$$\int_0^{R(\theta)} \left(\mu|\partial f(r)/\partial r|^2 + \tfrac{1}{2}v(r)|f(r)|^2\right) rdr \geq \mu\int_0^{R(\theta)} U(r)|f(r)|^2\, rdr, \tag{3.6}$$

where $R(\theta)$ denotes the distance of the origin to the boundary of $\mathcal{B}$ along the ray θ.

If $R(\theta) \leq R_0$ then (3.6) is trivial because the right side is zero while the left side is evidently nonnegative. (Here, $v \geq 0$ is used.)

If $R(\theta) > R_0$ for some given value of θ, consider the disc $\mathcal{D}(\theta) = \{\vec{x} \in \mathbb{R}^2 : 0 \leq |\vec{x}| \leq R(\theta)\}$ centered at the origin in $\mathbb{R}^2$ and of radius $R(\theta)$. Our

function f defines a spherically symmetric function, $\vec{x} \mapsto f(|\vec{x}|)$ on $\mathcal{D}(\theta)$, and (3.6) is equivalent to

$$\int_{\mathcal{D}(\theta)} \left(\mu |\nabla f(|\vec{x}|)|^2 + \frac{1}{2} v(|\vec{x}|) |f(|\vec{x}|)|^2 \right) d\vec{x} \geq \mu \int_{\mathcal{D}(\theta)} U(|\vec{x}|) |f(|\vec{x}|)|^2 d\vec{x}. \tag{3.7}$$

Now choose some $R \in (R_0,\ R(\theta))$ and note that the left side of (3.7) is not smaller than the same quantity with $\mathcal{D}(\theta)$ replaced by the smaller disc $\mathcal{D}_R = \{\vec{x} \in \mathbb{R}^2 \ :\ 0 \leq |\vec{x}| \leq R\}$. (Again, $v \geq 0$ is used.) We now minimize this integral over $\mathcal{D}_R$, fixing $f(R)$. This minimization problem leads to the zero energy scattering equation. Plugging in the solution and integrating by parts leads to

$$2\pi \int_0^{R(\theta)} \left(\mu |\partial f(r)/\partial r|^2 + \frac{1}{2} v(r) |f(r)|^2 \right) r dr \geq \frac{2\pi\mu}{\ln(R/a)} |f(R)|^2. \tag{3.8}$$

The proof is completed by multiplying both sides of (3.8) by $U(R) R \ln(R/a)$ and integrating with respect to R from R_0 to $R(\theta)$. ∎

As in Corollary 2.6, Lemma 3.1 can be used to bound the many body Hamiltonian H_N from below, as follows:

Corollary 3.2. *For any U as in Lemma 3.1 and any $0 < \varepsilon < 1$*

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu W \tag{3.9}$$

with $T_N = -\mu \sum_{i=1}^N \Delta_i$ and

$$W(\vec{x}_1, \ldots, \vec{x}_N) = \sum_{i=1}^N U\left(\min_{j, j\neq i} |\vec{x}_i - \vec{x}_j| . \right). \tag{3.10}$$

For U we choose the following functions, parameterized by $R > R_0$:

$$U_R(r) = \begin{cases} \nu(R)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise} \end{cases} \tag{3.11}$$

with $\nu(R)$ chosen so that

$$\int_{R_0}^R U_R(r) \ln(r/a) r\, dr = 1 \tag{3.12}$$

for all $R > R_0$, i.e.,

$$\nu(R) = \int_{R_0}^R \ln(r/a) r\, dr = \tfrac{1}{4} \left\{ R^2 \left(\ln(R^2/a^2) - 1 \right) - R_0^2 \left(\ln(R_0^2/a^2) - 1 \right) \right\}. \tag{3.13}$$

The nearest neighbor interaction (3.10) corresponding to U_R will be denoted W_R.

As in Subsection 2.2 we shall need estimates on the expectation value, $\langle W_R \rangle_0$, of W_R in the ground state of εT_N of (3.9) with Neumann boundary conditions. This is just the average value of W_R in a hypercube in $\mathbb{R}^{2N}$.

Besides the normalization factor $\nu(R)$, the computation involves the volume (area) of the support of U_R, which is

$$A(R) = \pi(R^2 - R_0^2). \tag{3.14}$$

In contrast to the three-dimensional situation the normalization factor $\nu(R)$ is not just a constant (R independent) multiple of $A(R)$; the factor $\ln(r/a)$ in (3.4) accounts for the more complicated expressions in the two-dimensional case. Taking into account that U_R is proportional to the characteristic function of a disc of radius R with a hole of radius R_0, the following inequalities for n particles in a box of side length ℓ are obtained by the same geometric reasoning as lead to (2.36), cf. [LY1]:

$$\langle W_R\rangle_0 \geq \frac{n}{\nu(R)}\left(1-\tfrac{2R}{\ell}\right)^2\left[1-(1-Q)^{(n-1)}\right] \tag{3.15}$$

$$\langle W_R\rangle_0 \leq \frac{n}{\nu(R)}\left[1-(1-Q)^{(n-1)}\right] \tag{3.16}$$

with

$$Q = A(R)/\ell^2 \tag{3.17}$$

being the relative volume occupied by the support of the potential U_R. Since $U_R^2 = \nu(R)^{-1}U_R$ we also have

$$\langle W_R^2\rangle_0 \leq \frac{n}{\nu(R)}\langle W_R\rangle_0. \tag{3.18}$$

As in [LY1] we estimate $[1-(1-Q)^{(n-1)}]$ by

$$(n-1)Q \geq \left[1-(1-Q)^{(n-1)}\right] \geq \frac{(n-1)Q}{1+(n-1)Q} \tag{3.19}$$

This gives

$$\langle W_R\rangle_0 \geq \frac{n(n-1)}{\nu(R)}\cdot\frac{Q}{1+(n-1)Q}, \tag{3.20}$$

$$\langle W_R\rangle_0 \leq \frac{n(n-1)}{\nu(R)}\cdot Q\,. \tag{3.21}$$

From Temple's inequality [T] we obtain like in (2.38) the estimate

$$E_0(n,\ell) \geq (1-\varepsilon)\langle W_R\rangle_0\left(1-\frac{\mu(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2)}{\langle W_R\rangle_0(E_1^{(0)}-\mu\langle W_R\rangle_0)}\right) \tag{3.22}$$

where

$$E_1^{(0)} = \frac{\varepsilon\mu}{\ell^2} \tag{3.23}$$

is the energy of the lowest excited state of εT_n. This estimate is valid for $E_1^{(0)}/\mu > \langle W_R\rangle_0$, i.e., it is important that ℓ is not too big.

Putting (3.20)–(3.22) together we obtain the estimate

$$E_0(n,\ell) \geq \frac{n(n-1)}{\ell^2}\frac{A(R)}{\nu(R)}K(n) \tag{3.24}$$

with

$$K(n) = (1-\varepsilon)\cdot \frac{(1-\frac{2R}{\ell})^2}{1+(n-1)Q}\cdot\left(1-\frac{n}{(\varepsilon\,\nu(R)/\ell^2)-n(n-1)\,Q}\right) \tag{3.25}$$

Note that Q depends on ℓ and R, and K depends on ℓ, R and ε besides n. We have here dropped the term $\langle W_R\rangle_0^2$ in the numerator in (3.22), which is appropriate for the purpose of a lower bound.

We note that K is monotonically decreasing in n, so for a given n we may replace $K(n)$ by $K(p)$ provided $p \geq n$. As explained in the previous section, (2.45)–(2.52), convexity of $n \mapsto n(n-1)$ together with superadditivity of $E_0(n,\ell)$ in n leads, for $p = 4\rho\ell^2$, to an estimate for the energy of N particles in the large box when the side length L is an integer multiple of ℓ:

$$E_0(N,L)/N \geq \frac{\rho A(R)}{\nu(R)}\left(1-\frac{1}{\rho\ell^2}\right)K(4\rho\ell^2) \tag{3.26}$$

with $\rho = N/L^2$.

Let us now look at the conditions on the parameters ε, R and ℓ that have to be met in order to obtain a lower bound with the same leading term as the upper bound (3.3).

From (3.13) we have

$$\frac{A(R)}{\nu(R)} = \frac{4\pi}{(\ln(R^2/a^2)-1)}\left(1-\mathrm{O}((R_0^2/R^2)\ln(R/R_0))\right) \tag{3.27}$$

We thus see that as long as $a < R < \rho^{-1/2}$ the logarithmic factor in the denominator in (3.27) has the right form for a lower bound. Moreover, for Temple's inequality the denominator in the third factor in (3.25) must be positive. With $n = 4\rho\ell^2$ and $\nu(R) \geq (\text{const.})R^2\ln(R^2/a^2)$ for $R \gg R_0$, this condition amounts to

$$(\text{const.})\varepsilon\ln(R^2/a^2)/\ell^2 > \rho^2\ell^4. \tag{3.28}$$

The relative error terms in (3.26) that have to be $\ll 1$ are

$$\varepsilon,\quad \frac{1}{\rho\ell^2},\quad \frac{R}{\ell},\quad \rho R^2,\quad \frac{\rho\ell^4}{\varepsilon R^2\ln(R^2/a^2)}. \tag{3.29}$$

We now choose

$$\varepsilon \sim |\ln(\rho a^2)|^{-1/5},\quad \ell \sim \rho^{-1/2}|\ln(\rho a^2)|^{1/10},\quad R \sim \rho^{-1/2}|\ln(\rho a^2)|^{-1/10} \tag{3.30}$$

Condition (3.28) is satisfied since the left side is $> (\text{const.})|\ln(\rho a^2)|^{3/5}$ and the right side is $\sim |\ln(\rho a^2)|^{2/5}$. The first three error terms in (3.29) are all of the same order, $|\ln(\rho a^2)|^{-1/5}$, the last is $\sim |\ln(\rho a^2)|^{-1/5}(\ln|\ln(\rho a^2)|)^{-1}$. With these choices, (3.26) thus leads to the following:

Theorem 3.3 (Lower bound). *For all N and L large enough such that $L > (\text{const.})\rho^{-1/2}|\ln(\rho a^2)|^{1/10}$ and $N > (\text{const.})|\ln(\rho a^2)|^{1/5}$ with $\rho = N/L^2$,*

the ground state energy with Neumann boundary condition satisfies

$$E_0(N,L)/N \geq \frac{4\pi\mu\rho}{|\ln(\rho a^2)|}\left(1 - \mathrm{O}(|\ln(\rho a^2)|^{-1/5})\right). \tag{3.31}$$

In combination with the upper bound (3.3) this also proves

Theorem 3.4 (Energy at low density in the thermodynamic limit).

$$\lim_{\rho a^2 \to 0} \frac{e_0(\rho)}{4\pi\mu\rho|\ln(\rho a^2)|^{-1}} = 1 \tag{3.32}$$

where $e_0(\rho) = \lim_{N\to\infty} E_0(N, \rho^{-1/2}N^{1/2})/N$. *This holds irrespective of boundary conditions.*

As in the three-dimensional case, Theorem 3.4 is also valid for an infinite range potential v provided that $v \geq 0$ and for some R we have $\int_R^\infty v(r)r\,dr < \infty$, which guarantees a finite scattering length.

4. Generalized Poincaré Inequalities

This section contains some lemmas that are of independent mathematical interest, but whose significance for the physics of the Bose gas may not be obvious at this point. They will, however, turn out to be important tools for the discussion of Bose-Einstein condensation (BEC) and superfluidity in the next section.

The classic Poincaré inequality [LLo] bounds the L^q-norm of a function, f, orthogonal to a given function g in a domain $\mathcal{K}$, in terms of some L^p-norm of its gradient in $\mathcal{K}$. For the proof of BEC we shall need a generalization of this inequality where the estimate is in terms of the gradient of f on a subset $\Omega \subset \mathcal{K}$ and a remainder that tends to zero with the volume of the complement $\Omega^c = \mathcal{K} \setminus \Omega$. For superfluidity it will be necessary to generalize this further by adding a vector potential to the gradient. This is the most complex of the lemmas because the other two can be derived directly from the classical Poincaré inequality using Hölder's inequality. The first lemma is the simplest variant and it is sufficient for the discussion of BEC in the case of a homogeneous gas. In this case the function g can be taken to be the constant function. The same holds for the second lemma, which will be used for the discussion of superfluidity in a homogeneous gas with periodic boundary conditions, but the modification of the gradient requires a more elaborate proof. The last lemma, that will be used for the discussion of BEC in the inhomogeneous case, is again a simple consequence of the classic Poincaré and Hölder inequalities. For a more comprehensive discussion of generalized Poincaré inequalities with further generalizations we refer to [LSeY7].

Lemma 4.1 (Generalized Poincaré inequality: Homogeneous case). *Let* $\mathcal{K} \subset \mathbb{R}^3$ *be a cube of side length* L, *and define the average of a function* $f \in L^1(\mathcal{K})$ *by*

$$\langle f \rangle_{\mathcal{K}} = \frac{1}{L^3}\int_{\mathcal{K}} f(\vec{x})\,d\vec{x}\,.$$

There exists a constant C such that for all measurable sets $\Omega \subset \mathcal{K}$ and all $f \in H^1(\mathcal{K})$ the inequality

$$\int_{\mathcal{K}} |f(\vec{x}) - \langle f \rangle_{\mathcal{K}}|^2 d\vec{x} \leq C \left(L^2 \int_{\Omega} |\nabla f(\vec{x})|^2 d\vec{x} + |\Omega^c|^{2/3} \int_{\mathcal{K}} |\nabla f(\vec{x})|^2 d\vec{x} \right) \tag{4.1}$$

holds. Here $\Omega^c = \mathcal{K} \setminus \Omega$, and $|\cdot|$ denotes the measure of a set. .

Proof. By scaling, it suffices to consider the case $L = 1$. Using the usual Poincaré-Sobolev inequality on $\mathcal{K}$ (see [LLo], Thm. 8.12), we infer that there exists a $C > 0$ such that

$$\begin{aligned} \|f - \langle f \rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})} &\leq \tfrac{1}{2} C \|\nabla f\|^2_{L^{6/5}(\mathcal{K})} \\ &\leq C \left(\|\nabla f\|^2_{L^{6/5}(\Omega)} + \|\nabla f\|^2_{L^{6/5}(\Omega^c)} \right) . \end{aligned} \tag{4.2}$$

Applying Hölder's inequality

$$\|\nabla f\|_{L^{6/5}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/3}$$

(and the analogue with Ω replaced by Ω^c), we see that (4.1) holds. ∎

In the next lemma $\mathcal{K}$ is again a cube of side length L, but we now replace the gradient ∇ by

$$\nabla_\varphi := \nabla + i(0, 0, \varphi/L), \tag{4.3}$$

where φ is a real parameter, and require periodic boundary conditions on $\mathcal{K}$.

Lemma 4.2 (Generalized Poincaré inequality with a vector potential). *For any $|\varphi| < \pi$ there are constants $c > 0$ and $C < \infty$ such that for all subsets $\Omega \subset \mathcal{K}$ and all functions $f \in H^1(\mathcal{K})$ with periodic boundary conditions on $\mathcal{K}$ the following estimate holds:*

$$\begin{aligned} \|\nabla_\varphi f\|^2_{L^2(\Omega)} \geq \frac{\varphi^2}{L^2} \|f\|^2_{L^2(\mathcal{K})} + \frac{c}{L^2} \|f - \langle f \rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})} \\ - C \left(\|\nabla_\varphi f\|^2_{L^2(\mathcal{K})} + \frac{1}{L^2} \|f\|^2_{L^2(\mathcal{K})} \right) \left(\frac{|\Omega|^c}{L^3} \right)^{1/2} . \end{aligned} \tag{4.4}$$

Here $|\Omega^c|$ is the volume of $\Omega^c = \mathcal{K} \setminus \Omega$, the complement of Ω in $\mathcal{K}$.

Proof. We shall derive (4.4) from a special form of this inequality that holds for all functions that are orthogonal to the constant function. Namely, for any positive $\alpha < 2/3$ and some constants $c > 0$ and $\widetilde{C} < \infty$ (depending only on α and $|\varphi| < \pi$) we claim that

$$\|\nabla_\varphi h\|^2_{L^2(\Omega)} \geq \frac{\varphi^2 + c}{L^2} \|h\|^2_{L^2(\mathcal{K})} - \widetilde{C} \left(\frac{|\Omega^c|}{L^3} \right)^{\alpha} \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})} , \tag{4.5}$$

provided $\langle 1, h \rangle_{\mathcal{K}} = 0$. (Remark: Eq. (4.5) holds also for $\alpha = 2/3$, but the proof is slightly more complicated in that case. See [LSeY7].) If (4.5) is

known the derivation of (4.4) is easy: For any f, the function $h = f - L^{-3}\langle 1, f\rangle_{\mathcal{K}}$ is orthogonal to 1. Moreover,

$$\begin{aligned}
\|\nabla_\varphi h\|^2_{L^2(\Omega)} &= \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})} - \|\nabla_\varphi h\|^2_{L^2(\Omega^c)} \\
&= \|\nabla_\varphi f\|^2_{L^2(\Omega)} - \frac{\varphi^2}{L^2}|\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2 \left(1 + \frac{|\Omega^c|}{L^3}\right) \\
&\quad + 2\frac{\varphi}{L}\mathrm{Re}\,\langle L^{-3/2}, f\rangle_{\mathcal{K}}\langle \nabla_\varphi f, L^{-3/2}\rangle_{\Omega^c} \\
&\leq \|\nabla_\varphi f\|^2_{L^2(\Omega)} - \frac{\varphi^2}{L^2}|\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2 \\
&\quad + \frac{|\varphi|}{L}\left(L\|\nabla_\varphi f\|^2_{L^2(\mathcal{K})} + \frac{1}{L}\|f\|^2_{L^2(\mathcal{K})}\right)\left(\frac{|\Omega^c|}{L^3}\right)^{1/2}
\end{aligned} \tag{4.6}$$

and

$$\begin{aligned}
\frac{\varphi^2 + c}{L^2}\|h\|^2_{L^2(\mathcal{K})} &= \frac{\varphi^2}{L^2}\left(\|f\|^2_{L^2(\mathcal{K})} - |\langle L^{-3/2}, f\rangle_{\mathcal{K}}|^2\right) \\
&\quad + \frac{c}{L^2}\|f - L^{-3}\langle 1, f\rangle_{\mathcal{K}}\|^2_{L^2(\mathcal{K})}\,.
\end{aligned} \tag{4.7}$$

Setting $\alpha = \frac{1}{2}$, using $\|\nabla_\varphi h\|_{L^2(\mathcal{K})} \leq \|\nabla_\varphi f\|_{L^2(\mathcal{K})}$ in the last term in (4.5) and combining (4.5), (4.6) and (4.7) gives (4.4) with $C = |\varphi| + \widetilde{C}$.

We now turn to the proof of (4.5). For simplicity we set $L = 1$. The general case follows by scaling. Assume that (4.5) is false. Then there exist sequences of constants $C_n \to \infty$, functions h_n with $\|h_n\|_{L^2(\mathcal{K})} = 1$ and $\langle 1, h_n\rangle_{\mathcal{K}} = 0$, and domains $\Omega_n \subset \mathcal{K}$ such that

$$\lim_{n\to\infty}\left\{\|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} + C_n|\Omega_n^c|^\alpha\|\nabla_\varphi h_n\|^2_{L^2(\mathcal{K})}\right\} \leq \varphi^2\,. \tag{4.8}$$

We shall show that this leads to a contradiction.

Since the sequence h_n is bounded in $L^2(\mathcal{K})$ it has a subsequence, denoted again by h_n, that converges weakly to some $h \in L^2(\mathcal{K})$ (i.e., $\langle g, h_n\rangle_{\mathcal{K}} \to \langle g, h\rangle_{\mathcal{K}}$ for all $g \in L^2(\mathcal{K})$). Moreover, by Hölder's inequality the $L^p(\Omega_n^c)$ norm $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)} = (\int_{\Omega_n^c}|\nabla_\varphi h(\vec{x})|^p d\vec{x})^{1/p}$ is bounded by $|\Omega_n^c|^{\alpha/2}\|\nabla_\varphi h_n\|_{L^2(\mathcal{K})}$ for $p = 2/(\alpha+1)$. From (4.8) we conclude that $\|\nabla_\varphi h_n\|_{L^p(\Omega_n^c)}$ is bounded and also that $\|\nabla_\varphi h_n\|_{L^p(\Omega_n)} \leq \|\nabla_\varphi h_n\|_{L^2(\Omega_n)}$ is bounded. Altogether, $\nabla_\varphi h_n$ is bounded in $L^p(\mathcal{K})$, and by passing to a further subsequence if necessary, we can therefore assume that $\nabla_\varphi h_n$ converges weakly in $L^p(\mathcal{K})$. The same applies to ∇h_n. Since $p = 2/(\alpha+1)$ with $\alpha < 2/3$ the hypotheses of the Rellich-Kondrashov Theorem [LLo, Thm 8.9] are fulfilled and consequently h_n converges *strongly* in $L^2(\mathcal{K})$ to h (i.e., $\|h - h_n\|_{L^2(\mathcal{K})} \to 0$). We shall now show that

$$\liminf_{n\to\infty}\|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} \geq \|\nabla_\varphi h\|^2_{L^2(\mathcal{K})}\,. \tag{4.9}$$

This will complete the proof because the h_n are normalized and orthogonal to 1 and the same holds for h by strong convergence. Hence the right side

of (4.9) is necessarily $> \varphi^2$, since for $|\varphi| < \pi$ the lowest eigenvalue of $-\nabla_\varphi^2$, with constant eigenfunction, is non-degenerate. This contradicts (4.8).

Eq. (4.9) is essentially a consequence of the weak lower semicontinuity of the L^2 norm, but the dependence on Ω_n leads to a slight complication. First, Eq. (4.8) and $C_n \to \infty$ clearly imply that $|\Omega_n^c| \to 0$, because $\|\nabla_\varphi h_n\|^2_{L^2(\mathcal{K})} > \varphi^2$. By choosing a subsequence we may assume that $\sum_n |\Omega_n^c| < \infty$. For some fixed N let $\widetilde{\Omega}_N = \mathcal{K} \setminus \cup_{n \geq N} \Omega_n^c$. Then $\tilde{\Omega}_N \subset \Omega_n$ for $n \geq N$. Since $\|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)}$ is bounded, $\nabla_\varphi h_n$ is also bounded in $L^2(\widetilde{\Omega}_N)$ and a subsequence of it converges weakly in $L^2(\widetilde{\Omega}_N)$ to $\nabla_\varphi h$. Hence

$$\liminf_{n\to\infty} \|\nabla_\varphi h_n\|^2_{L^2(\Omega_n)} \geq \liminf_{n\to\infty} \|\nabla_\varphi h_n\|^2_{L^2(\widetilde{\Omega}_N)} \geq \|\nabla_\varphi h\|^2_{L^2(\widetilde{\Omega}_N)} \,. \tag{4.10}$$

Since $\widetilde{\Omega}_N \subset \widetilde{\Omega}_{N+1}$ and $\cup_N \widetilde{\Omega}_N = \mathcal{K}$ (up to a set of measure zero), we can now let $N \to \infty$ on the right side of (4.10). By monotone convergence this converges to $\|\nabla_\varphi h\|^2_{L^2(\mathcal{K})}$. This proves (4.9) which, as remarked above, contradicts (4.8). ∎

The last lemma is a simple generalization of Lemma 4.1 with $\mathcal{K} \subset \mathbb{R}^m$ a bounded and connected set that is sufficiently nice so that the Poincaré-Sobolev inequality (see [LLo, Thm. 8.12]) holds on $\mathcal{K}$. In particular, this is the case if $\mathcal{K}$ satisfies the cone property [LLo] (e.g. if $\mathcal{K}$ is a rectangular box or a cube). Moreover, the constant function on $\mathcal{K}$ is here replaced by a more general bounded function.

Lemma 4.3 (Generalized Poincaré inequality: Inhomog. case). *For $d \geq 2$ let $\mathcal{K} \subset \mathbb{R}^d$ be as explained above, and let h be a bounded function with $\int_\mathcal{K} h = 1$. There exists a constant C (depending only on $\mathcal{K}$ and h) such that for all measurable sets $\Omega \subset \mathcal{K}$ and all $f \in H^1(\mathcal{K})$ with $\int_\mathcal{K} fh\, d\vec{x} = 0$, the inequality*

$$\int_\mathcal{K} |f(\vec{x})|^2 d\vec{x} \leq C \left(\int_\Omega |\nabla f(\vec{x})|^2 d\vec{x} + \left(\frac{|\Omega^c|}{|\mathcal{K}|} \right)^{2/d} \int_\mathcal{K} |\nabla f(\vec{x})|^2 d\vec{x} \right) \tag{4.11}$$

holds. Here $|\cdot|$ denotes the measure of a set, and $\Omega^c = \mathcal{K} \setminus \Omega$.

Proof. By the usual Poincaré-Sobolev inequality on $\mathcal{K}$ (see [LLo, Thm. 8.12]),

$$\begin{aligned} \|f\|^2_{L^2(\mathcal{K})} &\leq \tilde{C} \|\nabla f\|^2_{L^{2d/(d+2)}(\mathcal{K})} \\ &\leq 2\tilde{C} \left(\|\nabla f\|^2_{L^{2d/(d+2)}(\Omega)} + \|\nabla f\|^2_{L^{2d/(d+2)}(\Omega^c)} \right), \end{aligned} \tag{4.12}$$

if $d \geq 2$ and $\int_\mathcal{K} fh = 0$. Applying Hölder's inequality

$$\|\nabla f\|_{L^{2d/(d+2)}(\Omega)} \leq \|\nabla f\|_{L^2(\Omega)} |\Omega|^{1/d}$$

(and the analogue with Ω replaced by Ω^c), we see that (4.4) holds with $C = 2|\mathcal{K}|^{2/d}\tilde{C}$. ∎

5. Bose-Einstein Condensation and Superfluidity for Homogeneous Gases

5.1. **Bose-Einstein Condensation.** Bose-Einstein condensation (BEC) is the phenomenon of a macroscopic occupation of a single one-particle quantum state, discovered by Einstein for thermal equilibrium states of an ideal Bose gas at sufficiently low temperatures [E]. We are here concerned with interacting Bose gases, where the question of the existence of BEC is highly nontrivial even for the ground state. Due to the interaction the many body ground state is not a product of one-particle states but the concept of a macroscopic occupation of a single state acquires a precise meaning through the *one-particle density* matrix. Given the normalized ground state wave function this is the operator on $L^2(\mathbb{R}^d)$ ($d = 2$ or 3) given by the kernel

$$\gamma(\vec{x}, \vec{x}') = N \int \Psi_0(\vec{x}, \vec{X}) \Psi_0(\vec{x}', \vec{X}) d\vec{X} \,, \tag{5.1}$$

where we introduced the short hand notation

$$\vec{X} = (\vec{x}_2, \ldots, \vec{x}_N) \qquad \text{and} \quad d\vec{X} = \prod_{j=2}^{N} d\vec{x}_j. \tag{5.2}$$

Then $\int \gamma(\vec{x}, \vec{x}) d\vec{x} = \mathrm{Tr}\,[\gamma] = N$. BEC in the ground state means, by definition, that this operator has an eigenvalue of order N in the thermodynamic limit. Since γ is a positive kernel and, hopefully, translation invariant in the thermodynamic limit, the eigenfunction belonging to the largest eigenvalue must be the constant function $L^{-d/2}$. Therefore, another way to say that there is BEC in the ground state is that

$$\frac{1}{L^d} \int \int \gamma(\vec{x}, \vec{y}) d\vec{x} d\vec{y} = \mathrm{O}(N) \tag{5.3}$$

as $N \to \infty$, $L \to \infty$ with N/L^d fixed; more precisely Eq. (5.3) requires that there is a $c > 0$ such that the left side is $> cN$ for all large N. This is also referred to as *off-diagonal long range order*. Unfortunately, this is something that is frequently invoked but has so far never been proved for many body Hamiltonians with genuine interactions — except for one special case: hard core bosons on a lattice at half-filling (i.e., N = half the number of lattice sites). The proof is in [KLS] and [DLS].

The problem remains open after more than 75 years since the first investigations on the Bose gas [B, E]. Our construction in Section 2 shows that (in 3D) BEC exists on a length scale of order $\rho^{-1/3} Y^{-1/17}$ which, unfortunately, is not a 'thermodynamic' length like volume$^{1/3}$. The same remark applies to the 2D case of Section 3, where BEC is proved over a length scale $\rho^{-1/10} |\ln(\rho a^2)|^{1/10}$.

In a certain limit, however, one can prove (5.3), as has been shown in [LSe]. In this limit the interaction potential v is varied with N so that the ratio a/L of the scattering length to the box length is of order $1/N$, i.e., the

parameter Na/L is kept fixed. Changing a with N can be done by scaling, i.e., we write

$$v(|\vec{x}|) = \frac{1}{a^2} v_1(|\vec{x}|/a) \tag{5.4}$$

for some v_1 having scattering length 1, and vary a while keeping v_1 fixed. It is easily checked that the v so defined has scattering length a. It is important to note that, in the limit considered, a tends to zero (as $N^{-2/3}$ since $L = (N/\rho)^{1/3} \sim N^{1/3}$ for ρ fixed), and v becomes a *hard* potential of *short* range. This is the *opposite* of the usual mean field limit where the strength of the potential goes to zero while its range tends to infinity.

We shall refer to this as the *Gross-Pitaevskii (GP) limit* since Na/L will turn out to be the natural interaction parameter for inhomogeneous Bose gases confined in traps, that are described by the Gross-Pitaevskii equation discussed in Sections 6 and 7. Its significance for a homogeneous gas can also be seen by noting that Na/L is the ratio of ρa to $1/L^2$, i.e., in the GP limit the interaction energy per particle is of the same order of magnitude as the energy gap in the box, so that the interaction is still clearly visible, even though $a \to 0$. Note that $\rho a^3 \sim N^{-2}$ in the GP limit, so letting $N \to \infty$ with ρ fixed and Na/L fixed can be regarded as a *simultaneous thermodynamic and low density limit.* For simplicity, we shall here treat only the 3D case.

Theorem 5.1 (BEC in a dilute limit). *Assume that, as $N \to \infty$, $\rho = N/L^3$ and $g = Na/L$ stay fixed, and impose either periodic or Neumann boundary conditions for H. Then*

$$\lim_{N\to\infty} \frac{1}{N}\frac{1}{L^3} \int\int \gamma(\vec{x}, \vec{y}) d\vec{x} d\vec{y} = 1 \ . \tag{5.5}$$

The reason we do not deal with Dirichlet boundary conditions at this point should be clear from the discussion preceding the theorem: There would be an additional contribution $\sim 1/L^2$ to the energy, i.e. of the same order as the interaction energy, and the system would not be homogeneous any more. Dirichlet boundary conditions can, however, be treated with the methods of Section 7.

By scaling, the limit in Theorem 5.1 is equivalent to considering a Bose gas in a *fixed box* of side length $L = 1$, and keeping Na fixed as $N \to \infty$, i.e., $a \sim 1/N$. The ground state energy of the system is then, asymptotically, $N \times 4\pi Na$, and Theorem 5.1 implies that the one-particle reduced density matrix γ of the ground state converges, after division by N, to the projection onto the constant function. An analogous result holds true for inhomogeneous systems as will be discussed in Section 7.

The proof of Theorem 5.1 has two main ingredients. One is *localization of the energy* that is stated as Lemma 5.2 below. This lemma is a refinement of the energy estimates of Section 2.2 and says essentially that the kinetic energy of the ground state is concentrated in a subset of configuration space where at least one pair of particles is close together and whose volume tends to zero as $a \to 0$. The other is the generalized Poincaré inequality, Lemma

4.1 from which one deduces that the one particle density matrix is approximately constant if the kinetic energy is localized in a small set.

The localization lemma will be proved in a slightly more general version that is necessary for Theorem 5.1, namely with the gradient ∇ replaced by $\nabla_\varphi = \nabla + i(0,0,\varphi/L)$, cf. Eq. (4.3). We denote by H'_N the corresponding many-body Hamiltonian (2.1) with ∇_φ in place of ∇. This generalization will be used in the subsequent discussion of superfluidity, but a reader who wishes to focus on Theorem 5.1 only can simply ignore the φ and the reference to the diamagnetic inequality in the proof. We denote the gradient with respect to $\vec{x}_1$ by ∇_1, and the corresponding modified operator by $\nabla_{1,\varphi}$.

Lemma 5.2 (Localization of energy). *Let $\mathcal{K}$ be a box of side length L. For all symmetric, normalized wave functions $\Psi(\vec{x}_1,\ldots,\vec{x}_N)$ with periodic boundary conditions on $\mathcal{K}$, and for $N \geq Y^{-1/17}$,*

$$\frac{1}{N}\langle\Psi, H'_N\Psi\rangle \geq \left(1 - \text{const.}\, Y^{1/17}\right) \times\left(4\pi\mu\rho a + \mu\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\Omega_{\vec{X}}} d\vec{x}_1\left|\nabla_{1,\varphi}\Psi(\vec{x}_1,\vec{X})\right|^2\right), \tag{5.6}$$

where $\vec{X} = (\vec{x}_2,\ldots,\vec{x}_N)$, $d\vec{X} = \prod_{j=2}^N d\vec{x}_j$, and

$$\Omega_{\vec{X}} = \left\{\vec{x}_1 : \min_{j\geq 2}|\vec{x}_1 - \vec{x}_j| \geq R\right\} \tag{5.7}$$

with $R = aY^{-5/17}$.

Proof. Since Ψ is symmetric, the left side of (5.6) can be written as

$$\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\mathcal{K}} d\vec{x}_1\left[\mu\left|\nabla_{1,\varphi}\Psi(\vec{x}_1,\vec{X})\right|^2 + \tfrac{1}{2}\sum_{j\geq 2} v(|\vec{x}_1 - \vec{x}_j|)|\Psi(\vec{x}_1,\vec{X})|^2\right]. \tag{5.8}$$

For any $\varepsilon > 0$ and $R > 0$ this is

$$\geq \varepsilon T + (1-\varepsilon)(T^{\text{in}} + I) + (1-\varepsilon)T^{\text{out}}_\varphi\,, \tag{5.9}$$

with

$$T = \mu\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\mathcal{K}} d\vec{x}_1\left|\nabla_1|\Psi(\vec{x}_1,\vec{X})|\right|^2, \tag{5.10}$$

$$T^{\text{in}} = \mu\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\Omega^{\text{c}}_{\vec{X}}} d\vec{x}_1\left|\nabla_1|\Psi(\vec{x}_1,\vec{X})|\right|^2, \tag{5.11}$$

$$T^{\text{out}}_\varphi = \mu\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\Omega_{\vec{X}}} d\vec{x}_1\left|\nabla_{1,\varphi}\Psi(\vec{x}_1,\vec{X})\right|^2, \tag{5.12}$$

and

$$I = \tfrac{1}{2}\int_{\mathcal{K}^{N-1}} d\vec{X}\int_{\mathcal{K}} d\vec{x}_1\sum_{j\geq 2} v(|\vec{x}_1 - \vec{x}_j|)|\Psi(\vec{x}_1,\vec{X})|^2\,. \tag{5.13}$$

Here

$$\Omega^{\text{c}}_{\vec{X}} = \{\vec{x}_1 : |\vec{x}_1 - \vec{x}_j| < R \text{ for some } j \geq 2\} \tag{5.14}$$

is the complement of $\Omega_{\vec{X}}$, and the diamagnetic inequality [LLo] $|\nabla_\varphi f(\vec{x})|^2 \geq |\nabla|f(\vec{x})||^2$ has been used. The proof is completed by using the estimates used for the proof of Theorem 2.4, in particular (2.52) and (2.54)–(2.57), which tell us that for $\varepsilon = Y^{1/17}$ and $R = aY^{-5/17}$

$$\varepsilon T + (1-\varepsilon)(T^{\rm in} + I) \geq \big(1 - \text{const.}\, Y^{1/17}\big) 4\pi\mu\rho a \tag{5.15}$$

as long as $N \geq Y^{-1/17}$. ∎

Proof of Theorem 5.1. We combine Lemma 5.2 (with $\varphi = 0$ and hence $H'_N = H_N$) with Lemma 4.1 that gives a lower bound to the second term on the right side of (5.6). We thus infer that, for any symmetric Ψ with $\langle\Psi,\Psi\rangle = 1$ and for N large enough,

$$\begin{aligned}
&\frac{1}{N}\langle\Psi, H_N\Psi\rangle\big(1 - \text{const.}\, Y^{1/17}\big)^{-1} \\
&\geq 4\pi\mu\rho a - CY^{1/17}\Big(\frac{1}{L^2} - \frac{1}{N}\big\langle\Psi, \textstyle\sum_j \nabla_j^2\Psi\big\rangle\Big) \\
&\quad + \frac{c}{L^2}\int_{\mathcal{K}^{N-1}} d\vec{X} \int_{\mathcal{K}} d\vec{x}_1 \Big|\Psi(\vec{x}_1, \vec{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}} d\vec{x}\Psi(\vec{x}, \vec{X})\big]\Big|^2 ,
\end{aligned} \tag{5.16}$$

where we used that $|\Omega^c| \leq \frac{4\pi}{3}NR^3 = \text{const.}\, L^3 Y^{2/17}$. Since the kinetic energy, divided by N, is certainly bounded independent of N, as the upper bound (2.14) shows, and since the upper and the lower bound to E_0 agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function Ψ_0 of H_N

$$\lim_{N\to\infty} \int_{\mathcal{K}^{N-1}} d\vec{X} \int_{\mathcal{K}} d\vec{x}_1 \Big|\Psi_0(\vec{x}_1, \vec{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}} d\vec{x}\Psi_0(\vec{x}, \vec{X})\big]\Big|^2 = 0 . \tag{5.17}$$

This proves (5.5), since

$$\begin{aligned}
&\int_{\mathcal{K}^{N-1}} d\vec{X} \int_{\mathcal{K}} d\vec{x}_1 \Big|\Psi_0(\vec{x}_1, \vec{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}} d\vec{x}\Psi_0(\vec{x}, \vec{X})\big]\Big|^2 \\
&= 1 - \frac{1}{NL^3}\int_{\mathcal{K}\times\mathcal{K}} \gamma(\vec{x}, \vec{x}')d\vec{x}d\vec{x}' .
\end{aligned} \tag{5.18}$$

∎

5.2. **Superfluidity.** The phenomenological two-fluid model of superfluidity (see, e.g., [TT]) is based on the idea that the particle density ρ is composed of two parts, the density $\rho_{\rm s}$ of the inviscid superfluid and the normal fluid density $\rho_{\rm n}$. If an external velocity field is imposed on the fluid (for instance by moving the walls of the container) only the viscous normal component responds to the velocity field, while the superfluid component stays at rest. In accord with these ideas the superfluid density in the ground state is often defined as follows [HoM]: Let E_0 denote the ground state energy of the

system in the rest frame and E_0' the ground state energy, measured in the moving frame, when a velocity field $\mathbf{v}$ is imposed. Then for small $\mathbf{v}$

$$\frac{E_0'}{N} = \frac{E_0}{N} + (\rho_s/\rho)\tfrac{1}{2}m\mathbf{v}^2 + O(|\mathbf{v}|^4) \tag{5.19}$$

where N is the particle number and m the particle mass. At positive temperatures the ground state energy should be replaced by the free energy. (Remark: It is important here that (5.19) holds uniformly for all large N; i.e., that the error term $O(|\mathbf{v}|^4)$ can be bounded independently of N. For fixed N and a finite box, Eq. (5.19) with $\rho_s/\rho = 1$ always holds for a Bose gas with an arbitrary interaction if $\mathbf{v}$ is small enough, owing to the discreteness of the energy spectrum.[1] There are other definitions of the superfluid density that may lead to different results [PrSv], but this is the one we shall use here and shall not dwell on this issue since it is not clear that there is a "one-size-fits-all" definition of superfluidity. For instance, in the definition we use here the ideal Bose gas is a perfect superfluid in its ground state, whereas the definition of Landau in terms of a linear dispersion relation of elementary excitations would indicate otherwise. Our main result is that with the definition adopted here there is 100% superfluidity in the ground state of a 3D Bose gas in the GP limit explained in the previous subsection.

One of the unresolved issues in the theory of superfluidity is its relation to Bose-Einstein condensation (BEC). It has been argued that in general neither condition is necessary for the other (c.f., e.g., [H, ABCG, KT]), but in the case considered here, i.e., the GP limit of a 3D gas, we show that 100% BEC into the constant wave function (in the rest frame) prevails even if an external velocity field is imposed. A simple example illustrating the fact that BEC is not necessary for superfluidity is the 1D hard-core Bose gas. This system is well known to have a spectrum like that of an ideal Fermi gas [Gi] (see also Section 8), and it is easy to see that it is superfluid in its ground state in the sense of (5.19). On the other hand, it has no BEC [Le, PiSt]. The definition of the superfluid velocity as the gradient of the phase of the condensate wave function [HoM, Bm] is clearly not applicable in such cases.

We consider a Bose gas with the Hamiltonian (2.1) in a box $\mathcal{K}$ of side length L, assuming periodic boundary conditions in all three coordinate directions. Imposing an external velocity field $\mathbf{v} = (0, 0, \pm|\mathbf{v}|)$ means that the momentum operator $\mathbf{p} = -i\hbar\nabla$ is replaced by by $\mathbf{p} - m\mathbf{v}$, retaining the

[1]The ground state with $\mathbf{v} = 0$ remains an eigenstate of the Hamiltonian with arbitrary $\mathbf{v}$ (but not necesssarily a ground state) since its total momentum is zero. Its energy is $\frac{1}{2}mN\mathbf{v}^2$ above the ground state energy for $\mathbf{v} = 0$. Since in a finite box the spectrum of the Hamiltonian for arbitrary $\mathbf{v}$ is discrete and the energy gap above the ground state is bounded away from zero for $\mathbf{v}$ small, the ground state for $\mathbf{v} = 0$ is at the same time the ground state of the Hamiltonian with $\mathbf{v}$ if $\frac{1}{2}mN\mathbf{v}^2$ is smaller than the gap.

periodic boundary conditions. The Hamiltonian in the moving frame is thus

$$H'_N = -\mu \sum_{j=1}^{N} \nabla_{j,\varphi}^2 + \sum_{1\le i<j\le N} v(|\vec{x}_i - \vec{x}_j|) \,, \tag{5.20}$$

where $\nabla_{j,\varphi} = \nabla_j + i(0,0,\varphi/L)$ and the dimensionless phase φ is connected to the velocity $\mathbf{v}$ by

$$\varphi = \frac{\pm|\mathbf{v}|Lm}{\hbar} \,. \tag{5.21}$$

Let $E_0(N,a,\varphi)$ denote the ground state energy of (5.20) with periodic boundary conditions. Obviously it is no restriction to consider only the case $-\pi \le \varphi \le \pi$, since E_0 is periodic in φ with period 2π (see Remark 1 below). For Ψ_0 the ground state of H'_N, let γ_N be its one-particle reduced density matrix. We are interested in the *Gross-Pitaevskii* (GP) limit $N \to \infty$ with Na/L fixed. We also fix the box size L. This means that a should vary like $1/N$ which, as explained in the previous subsection, can be achieved by writing $v(r) = a^{-2}v_1(r/a)$, where v_1 is a fixed potential with scattering length 1, while a changes with N.

Theorem 5.3 (Superfluidity and BEC of homogeneous gas). *For* $|\varphi| \le \pi$

$$\lim_{N\to\infty} \frac{E_0(N,a,\varphi)}{N} = 4\pi\mu a\rho + \mu\frac{\varphi^2}{L^2} \tag{5.22}$$

in the limit $N \to \infty$ *with* Na/L *and* L *fixed. Here* $\rho = N/L^3$, *so* $a\rho$ *is fixed too. In the same limit, for* $|\varphi| < \pi$,

$$\lim_{N\to\infty} \frac{1}{N}\gamma_N(\vec{x},\vec{x}') = \frac{1}{L^3} \tag{5.23}$$

in trace class norm, i.e., $\lim_{N\to\infty} \mathrm{Tr}\left[\,\left|\gamma_N/N - |L^{-3/2}\rangle\langle L^{-3/2}|\,\right|\right] = 0$.

Note that, by the definition (5.19) of ρ_s and Eq. (5.21), Eq. (5.22) means that $\rho_s = \rho$, i.e., there is 100% superfluidity. For $\varphi = 0$, Eq. (5.22) follows from Eq. 2.8, while (5.23) for $\varphi = 0$ is the BEC of Theorem 5.1.[2]

Remarks. 1. By a unitary gauge transformation,

$$\big(U\Psi\big)(\vec{x}_1,\ldots,\vec{x}_N) = e^{i\varphi(\sum_i z_i)/L}\,\Psi(\vec{x}_1,\ldots,\vec{x}_N) \,, \tag{5.24}$$

the passage from (2.1) to (5.20) is equivalent to replacing periodic boundary conditions in a box by the *twisted boundary condition*

$$\Psi(\vec{x}_1 + (0,0,L),\vec{x}_2,\ldots,\vec{x}_N) = e^{i\varphi}\Psi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N) \tag{5.25}$$

in the direction of the velocity field, while retaining the original Hamiltonian (2.1).

[2]The convention in Theorem 5.1, where ρ and Na/L stay fixed, is different from the one employed here, where L and Na/L are fixed, but these two conventions are clearly equivalent by scaling.

2. The criterion $|\varphi| \leq \pi$ means that $|\mathbf{v}| \leq \pi\hbar/(mL)$. The corresponding energy $\frac{1}{2}m(\pi\hbar/(mL))^2$ is the gap in the excitation spectrum of the one-particle Hamiltonian in the finite-size system.

3. The reason that we have to restrict ourselves to $|\varphi| < \pi$ in the second part of Theorem 5.3 is that for $|\varphi| = \pi$ there are two ground states of the operator $(\nabla + \mathrm{i}\varphi/L)^2$ with periodic boundary conditions. All we can say in this case is that there is a subsequence of γ_N that converges to a density matrix of rank ≤ 2, whose range is spanned by these two functions

Proof of Theorem 5.3. As in the proof of Theorem 5.1 we combine the localization Lemma 5.2, this time with $\varphi \neq 0$, and a generalized Poincaré inequality, this time Lemma 4.2. We thus infer that, for any symmetric Ψ with $\langle\Psi, \Psi\rangle = 1$ and for N large enough,

$$\begin{aligned}
&\frac{1}{N}\langle\Psi, H'_N\Psi\rangle\big(1 - \text{const.}\, Y^{1/17}\big)^{-1} \\
&\geq 4\pi\mu\rho a + \mu\frac{\varphi^2}{L^2} - CY^{1/17}\Big(\frac{1}{L^2} - \frac{1}{N}\big\langle\Psi, \textstyle\sum_j \nabla^2_{j,\varphi}\Psi\big\rangle\Big) \\
&\quad + \frac{c}{L^2}\int_{\mathcal{K}^{N-1}} d\vec{X} \int_{\mathcal{K}} d\vec{x}_1 \Big|\Psi(\vec{x}_1, \vec{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}} d\vec{x}\Psi(\vec{x}, \vec{X})\big]\Big|^2 ,
\end{aligned}$$

where we used that $|\Omega^c| \leq \frac{4\pi}{3}NR^3 = \text{const.}\, L^3Y^{2/17}$. From this we can infer two things. First, since the kinetic energy, divided by N, is certainly bounded independently of N, as the upper bound shows, we get that

$$\liminf_{N\to\infty} \frac{E_0(N, a, \varphi)}{N} \geq 4\pi\mu\rho a + \mu\frac{\varphi^2}{L^2} \tag{5.26}$$

for any $|\varphi| < \pi$. By continuity this holds also for $|\varphi| = \pi$, proving (5.22). (To be precise, $E_0/N - \mu\varphi^2L^{-2}$ is concave in φ, and therefore stays concave, and in particular continuous, in the limit $N \to \infty$.) Secondly, since the upper and the lower bounds to E_0 agree in the limit considered, the positive last term in (5.16) has to vanish in the limit. I.e., we get that for the ground state wave function Ψ_0 of H'_N

$$\lim_{N\to\infty} \int_{\mathcal{K}^{N-1}} d\vec{X} \int_{\mathcal{K}} d\vec{x}_1 \Big|\Psi_0(\vec{x}_1, \vec{X}) - L^{-3}\big[\textstyle\int_{\mathcal{K}} d\vec{x}\Psi_0(\vec{x}, \vec{X})\big]\Big|^2 = 0 . \tag{5.27}$$

Using again (5.18), this proves (5.23) in a weak sense. As explained in [LSe, LSSY], this suffices for the convergence $N^{-1}\gamma_N \to |L^{-3/2}\rangle\langle L^{-3/2}|$ in trace class norm. ∎

Theorem 5.3 can be generalized in various ways to a physically more realistic setting, for example replacing the periodic box by a cylinder centered at the origin. We shall comment on such extensions at the end of Section 7.

6. Gross-Pitaevskii Equation for Trapped Bosons

In the recent experiments on Bose condensation (see, e.g., [KD]), the particles are confined at very low temperatures in a 'trap' where the particle

density is *inhomogeneous*, contrary to the case of a large 'box', where the density is essentially uniform. We model the trap by a slowly varying confining potential V, with $V(\vec{x}) \to \infty$ as $|\vec{x}| \to \infty$. The Hamiltonian becomes

$$H = \sum_{i=1}^{N} \{-\mu\Delta_i + V(\vec{x}_i)\} + \sum_{1\le i<j\le N} v(|\vec{x}_i - \vec{x}_j|)\ . \tag{6.1}$$

Shifting the energy scale if necessary we can assume that V is nonnegative. The ground state energy, $\hbar\omega$, of $-\mu\Delta + V(\vec{x})$ is a natural energy unit and the corresponding length unit, $\sqrt{\hbar/(m\omega)} = \sqrt{2\mu/(\hbar\omega)} \equiv L_{\rm osc}$, is a measure of the extension of the trap.

In the sequel we shall be considering a limit where $a/L_{\rm osc}$ tends to zero while $N \to \infty$. Experimentally $a/L_{\rm osc}$ can be changed in two ways: One can either vary $L_{\rm osc}$ or a. The first alternative is usually simpler in practice but very recently a direct tuning of the scattering length itself has also been shown to be feasible [CCRCW]. Mathematically, both alternatives are equivalent, of course. The first corresponds to writing $V(\vec{x}) = L_{\rm osc}^{-2} V_1(\vec{x}/L_{\rm osc})$ and keeping V_1 and v fixed. The second corresponds to writing the interaction potential as $v(|\vec{x}|) = a^{-2} v_1(|\vec{x}|/a)$ like in (5.4), where v_1 has unit scattering length, and keeping V and v_1 fixed. This is equivalent to the first, since for given V_1 and v_1 the ground state energy of (6.1), measured in units of $\hbar\omega$, depends only on N and $a/L_{\rm osc}$. In the dilute limit when a is much smaller than the mean particle distance, the energy becomes independent of v_1.

We choose $L_{\rm osc}$ as a length unit. The energy unit is $\hbar\omega = 2\mu L_{\rm osc}^{-2} = 2\mu$. Moreover, we find it convenient to regard V and v_1 as fixed. This justifies the notion $E_0(N, a)$ for the quantum mechanical ground state energy.

The idea is now to use the information about the thermodynamic limiting energy of the dilute Bose gas in a box to find the ground state energy of (6.1) in an appropriate limit. This has been done in [LSeY1, LSeY2] and in this section we give an account of this work. As we saw in Sections 2 and 3 there is a difference in the ρ dependence between two and three dimensions, so we can expect a related difference now. We discuss 3D first.

6.1. **Three Dimensions.** Associated with the quantum mechanical ground state energy problem is the Gross-Pitaevskii (GP) energy functional [Gr1, Gr2, Pi]

$$\mathcal{E}^{\rm GP}[\phi] = \int_{\mathbb{R}^3} \left(\mu|\nabla\phi|^2 + V|\phi|^2 + 4\pi\mu a|\phi|^4\right) d\vec{x} \tag{6.2}$$

with the subsidiary condition

$$\int_{\mathbb{R}^3} |\phi|^2 = N. \tag{6.3}$$

As before, $a > 0$ is the scattering length of v. The corresponding energy is

$$E^{\rm GP}(N, a) = \inf_{\int|\phi|^2=N} \mathcal{E}^{\rm GP}[\phi] = \mathcal{E}^{\rm GP}[\phi^{\rm GP}], \tag{6.4}$$

with a unique, positive ϕ^{GP}. The existence of the minimizer ϕ^{GP} is proved by standard techniques and it can be shown to be continuously differentiable, see [LSeY1], Sect. 2 and Appendix A. The minimizer depends on N and a, of course, and when this is important we denote it by $\phi^{\mathrm{GP}}_{N,a}$.

The variational equation satisfied by the minimizer is the *GP equation*

$$-\mu\Delta\phi^{\mathrm{GP}}(\vec{x}) + V(\vec{x})\phi^{\mathrm{GP}}(\vec{x}) + 8\pi\mu a\phi^{\mathrm{GP}}(\vec{x})^3 = \mu^{\mathrm{GP}}\phi^{\mathrm{GP}}(\vec{x}), \tag{6.5}$$

where μ^{GP} is the chemical potential, given by

$$\mu^{\mathrm{GP}} = dE^{\mathrm{GP}}(N,a)/dN = E^{\mathrm{GP}}(N,a)/N + (4\pi\mu a/N)\int |\phi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x}. \tag{6.6}$$

The GP theory has the following scaling property:

$$E^{\mathrm{GP}}(N,a) = NE^{\mathrm{GP}}(1,Na), \tag{6.7}$$

and

$$\phi^{\mathrm{GP}}_{N,a}(\vec{x}) = N^{1/2}\phi^{\mathrm{GP}}_{1,Na}(\vec{x}). \tag{6.8}$$

Hence we see that the relevant parameter in GP theory is the combination Na.

We now turn to the relation of E^{GP} and ϕ^{GP} to the quantum mechanical ground state. If $v = 0$, then the ground state of (6.1) is

$$\Psi_0(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^N \phi_0(\vec{x}_i)$$

with ϕ_0 the normalized ground state of $-\mu\Delta + V(\vec{x})$. In this case clearly $\phi^{\mathrm{GP}} = \sqrt{N}\ \phi_0$, and then $E^{\mathrm{GP}} = N\hbar\omega = E_0$. In the other extreme, if $V(\vec{x}) = 0$ for $\vec{x}$ inside a large box of volume L^3 and $V(\vec{x}) = \infty$ otherwise, then $\phi^{\mathrm{GP}} \approx \sqrt{N/L^3}$ and we get $E^{\mathrm{GP}}(N,a) = 4\pi\mu aN^2/L^3$, which is the previously considered energy E_0 for the homogeneous gas in the low density regime. (In this case, the gradient term in $\mathcal{E}^{\mathrm{GP}}$ plays no role.)

In general, we expect that for *dilute* gases in a suitable limit

$$E_0 \approx E^{\mathrm{GP}} \quad \text{and} \quad \rho^{\mathrm{QM}}(\vec{x}) \approx \left|\phi^{\mathrm{GP}}(\vec{x})\right|^2 \equiv \rho^{\mathrm{GP}}(\vec{x}), \tag{6.9}$$

where the quantum mechanical particle density in the ground state is defined by

$$\rho^{\mathrm{QM}}(\vec{x}) = N\int |\Psi_0(\vec{x},\vec{x}_2,\ldots,\vec{x}_N)|^2 d\vec{x}_2\cdots d\vec{x}_N. \tag{6.10}$$

Dilute means here that

$$\bar{\rho}a^3 \ll 1, \tag{6.11}$$

where

$$\bar{\rho} = \frac{1}{N}\int |\rho^{\mathrm{GP}}(\vec{x})|^2 d\vec{x} \tag{6.12}$$

is the *mean density.*

The limit in which (6.9) can be expected to be true should be chosen so that *all three* terms in $\mathcal{E}^{\mathrm{GP}}$ make a contribution. The scaling relations (6.7) and (6.8) indicate that fixing Na as $N \to \infty$ is the right thing to do (and this is quite relevant since experimentally N can be quite large, 10^6 and more, and Na can range from about 1 to 10^4 [DGPS]). Fixing Na (which we refer

to as the GP case) also means that we really are dealing with a dilute limit, because the mean density $\bar{\rho}$ is then of the order N (since $\bar{\rho}_{N,a} = N\bar{\rho}_{1,Na}$) and hence

$$a^3\bar{\rho} \sim N^{-2}. \tag{6.13}$$

The precise statement of (6.9) is:

Theorem 6.1 (GP limit of the QM ground state energy and density). *If $N \to \infty$ with Na fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{GP}}(N,a)} = 1, \tag{6.14}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\mathrm{QM}}_{N,a}(\vec{x}) = \left|\phi^{\mathrm{GP}}_{1,Na}(\vec{x})\right|^2 \tag{6.15}$$

in the weak L^1-sense.

Convergence can not only be proved for the ground state energy and density, but also for the individual energy components:

Theorem 6.2 (Asymptotics of the energy components). *Let ψ_0 denote the solution to the zero-energy scattering equation for v (under the boundary condition $\lim_{|\vec{x}|\to\infty}\psi_0(\vec{x}) = 1$) and $s = \int|\nabla\psi_0|^2/(4\pi a)$. Then $0 < s \leq 1$ and, in the same limit as in Theorem 6.1 above,*

$$\lim_{N\to\infty}\int|\nabla_{\vec{x}_1}\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\, d\vec{X}$$

$$= \int|\nabla\phi^{\mathrm{GP}}_{1,Na}(\vec{x})|^2 d\vec{x} + 4\pi Nas\int|\phi^{\mathrm{GP}}_{1,Na}(\vec{x})|^4 d\vec{x}, \tag{6.16a}$$

$$\lim_{N\to\infty}\int V(\vec{x}_1)|\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\, d\vec{X} = \int V(\vec{x})|\phi^{\mathrm{GP}}_{1,Na}(\vec{x})|^2 d\vec{x}, \tag{6.16b}$$

$$\lim_{N\to\infty}\tfrac{1}{2}\sum_{j=2}^{N}\int v(|\vec{x}_1-\vec{x}_j|)|\Psi_0(\vec{x}_1,\vec{X})|^2 d\vec{x}_1\, d\vec{X}$$

$$= (1-s)4\pi Na\int|\phi^{\mathrm{GP}}_{1,Na}(\vec{x})|^4 d\vec{x}. \tag{6.16c}$$

Here we introduced again the short hand notation (5.2). Theorem 6.2 is a simple consequence of Theorem 6.1 by variation with respect to the different components of the energy, as was also noted in [CS2]. More precisely, Eq. (6.14) can be written as

$$\lim_{N\to\infty}\frac{1}{N}E_0(N,a) = E^{\mathrm{GP}}(1,Na). \tag{6.17}$$

The ground state energy is a concave function of the mass parameter μ, so it is legitimate to differentiate both sides of (6.17) with respect to μ. In doing so, it has to be noted that Na depends on μ through the scattering length. Using (2.13) one sees that

$$\frac{d(\mu a)}{d\mu} = \frac{1}{4\pi}\int|\nabla\psi_0|^2 d\vec{x} \tag{6.18}$$

by the Feynman-Hellmann principle, since ψ_0 minimizes the left side of (2.13).

We remark that in the case of a two-dimensional Bose gas, where the relevant parameter to be kept fixed in the GP limit is $N/|\ln(a^2\bar{\rho}_N)|$ (c.f. Sections 3 and 6.2.), the parameter s in Theorem 6.2 can be shown to be always equal to 1. I.e., in 2D the interaction energy is purely kinetic in the GP limit (see [CS1]).

To describe situations where Na is very large, it is appropriate to consider a limit where, as $N \to \infty$, $a \gg N^{-1}$, i.e. $Na \to \infty$, but still $\bar{\rho}a^3 \to 0$. In this case, the gradient term in the GP functional becomes negligible compared to the other terms and the so-called *Thomas-Fermi (TF) functional*

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{\mathbb{R}^3} \left(V\rho + 4\pi\mu a\rho^2\right) d\vec{x} \tag{6.19}$$

arises. (Note that this functional has nothing to do with the fermionic theory invented by Thomas and Fermi in 1927, except for a certain formal analogy.) It is defined for nonnegative functions ρ on $\mathbb{R}^3$. Its ground state energy E^{TF} and density ρ^{TF} are defined analogously to the GP case. (The TF functional is especially relevant for the two-dimensional Bose gas. There a has to decrease exponentially with N in the GP limit, so the TF limit is more adequate; see Subsection 6.2 below).

Our second main result of this section is that minimization of (6.19) reproduces correctly the ground state energy and density of the many-body Hamiltonian in the limit when $N \to \infty$, $a^3\bar{\rho} \to 0$, but $Na \to \infty$ (which we refer to as the TF case), provided the external potential is reasonably well behaved. We will assume that V is asymptotically equal to some function W that is homogeneous of some order $s > 0$, i.e., $W(\lambda\vec{x}) = \lambda^s W(\vec{x})$ for all $\lambda > 0$, and locally Hölder continuous (see [LSeY2] for a precise definition). This condition can be relaxed, but it seems adequate for most practical applications and simplifies things considerably.

Theorem 6.3 (TF limit of the QM ground state energy and density). *Assume that V satisfies the conditions stated above. If $g \equiv Na \to \infty$ as $N \to \infty$, but still $a^3\bar{\rho} \to 0$, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{TF}}(N,a)} = 1, \tag{6.20}$$

and

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho^{\mathrm{QM}}_{N,a}(g^{1/(s+3)}\vec{x}) = \tilde{\rho}^{\mathrm{TF}}_{1,1}(\vec{x}) \tag{6.21}$$

in the weak L^1-sense, where $\tilde{\rho}^{\mathrm{TF}}_{1,1}$ is the minimizer of the TF functional under the condition $\int \rho = 1$, $a = 1$, and with V replaced by W.

In the following, we will present the essentials of the proofs Theorems 6.1 and 6.3. We will derive appropriate upper and lower bounds on the ground state energy E_0.

The proof of the lower bound in Theorem 6.1 presented here is a modified version of (and partly simpler than) the original proof in [LSeY1].

The convergence of the densities follows from the convergence of the energies in the usual way by variation with respect to the external potential. For simplicity, we set $\mu \equiv 1$ in the following.

Proof of Theorems 6.1 and 6.3. Part 1: Upper bound to the QM energy. To derive an upper bound on E_0 we use a generalization of a trial wave function of Dyson [D1], who used this function to give an upper bound on the ground state energy of the homogeneous hard core Bose gas (c.f. Section 2.1). It is of the form

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = \prod_{i=1}^{N} \phi^{\mathrm{GP}}(\vec{x}_i) F(\vec{x}_1, \ldots, \vec{x}_N), \tag{6.22}$$

where F is constructed in the following way:

$$F(\vec{x}_1, \ldots, \vec{x}_N) = \prod_{i=1}^{N} f(t_i(\vec{x}_1, \ldots, \vec{x}_i)), \tag{6.23}$$

where $t_i = \min\{|\vec{x}_i - \vec{x}_j|, 1 \leq j \leq i-1\}$ is the distance of $\vec{x}_i$ to its *nearest neighbor* among the points $\vec{x}_1, \ldots, \vec{x}_{i-1}$, and f is a function of $r \geq 0$. As in (2.20) we choose it to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } r < b \\ 1 & \text{for } r \geq b, \end{cases} \tag{6.24}$$

where f_0 is the solution of the zero energy scattering equation (2.3) and b is some cut-off parameter of order $b \sim \bar{\rho}^{-1/3}$. The function (6.22) is not totally symmetric, but for an upper bound it is nevertheless an acceptable test wave function since the bosonic ground state energy is equal to the *absolute* ground state energy.

The result of a somewhat lengthy computation (see [LSeY1] for details) is the upper bound

$$E_0(N, a) \leq E^{\mathrm{GP}}(N, a) \left(1 + O(a\bar{\rho}^{1/3})\right). \tag{6.25}$$

Part 2: Lower bound to the QM energy, GP case. To obtain a lower bound for the QM ground state energy the strategy is to divide space into boxes and use the estimate on the homogeneous gas, given in Theorem 2.4, in each box with *Neumann* boundary conditions. One then minimizes over all possible divisions of the particles among the different boxes. This gives a lower bound to the energy because discontinuous wave functions for the quadratic form defined by the Hamiltonian are now allowed. We can neglect interactions among particles in different boxes because $v \geq 0$. Finally, one lets the box size tend to zero. However, it is not possible to simply approximate V by a constant potential in each box. To see this consider the case of noninteracting particles, i.e., $v = 0$ and hence $a = 0$. Here $E_0 = N\hbar\omega$, but a 'naive' box method gives only $\min_{\vec{x}} V(\vec{x})$ as lower bound, since it clearly

pays to put all the particles with a constant wave function in the box with the lowest value of V.

For this reason we start by separating out the GP wave function in each variable and write a general wave function Ψ as

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = \prod_{i=1}^{N} \phi^{\mathrm{GP}}(\vec{x}_i) F(\vec{x}_1, \ldots, \vec{x}_N). \tag{6.26}$$

Here $\phi^{\mathrm{GP}} = \phi^{\mathrm{GP}}_{N,a}$ is normalized so that $\int |\phi^{\mathrm{GP}}|^2 = N$. Eq. (6.26) defines F for a given Ψ because ϕ^{GP} is everywhere strictly positive, being the ground state of the operator $-\Delta + V + 8\pi a|\phi^{\mathrm{GP}}|^2$. We now compute the expectation value of H in the state Ψ. Using partial integration and the variational equation (6.5) for ϕ^{GP}, we see that

$$\frac{\langle \Psi | H \Psi \rangle}{\langle \Psi | \Psi \rangle} - E^{\mathrm{GP}}(N, a) = 4\pi a \int |\rho^{\mathrm{GP}}|^2 + Q(F), \tag{6.27}$$

with

$$Q(F) = \sum_{i=1}^{N} \frac{\int \prod_{k=1}^{N} \rho^{\mathrm{GP}}(\vec{x}_k) \left(|\nabla_i F|^2 + \left[\frac{1}{2} \sum_{j \neq i} v(|\vec{x}_i - \vec{x}_j|) - 8\pi a \rho^{\mathrm{GP}}(\vec{x}_i) \right] |F|^2 \right)}{\int \prod_{k=1}^{N} \rho^{\mathrm{GP}}(\vec{x}_k) |F|^2}. \tag{6.28}$$

We recall that $\rho^{\mathrm{GP}}(\vec{x}) = |\phi^{\mathrm{GP}}_{N,a}(\vec{x})|^2$. For computing the ground state energy of H we have to minimize the normalized quadratic form Q. Compared to the expression for the energy involving Ψ itself we have thus obtained the replacements

$$V(\vec{x}) \to -8\pi a \rho^{\mathrm{GP}}(\vec{x}) \quad \text{and} \quad \prod_{i=1}^{N} d\vec{x}_i \to \prod_{i=1}^{N} \rho^{\mathrm{GP}}(\vec{x}_i) d\vec{x}_i \,. \tag{6.29}$$

We now use the box method on *this* problem. More precisely, labeling the boxes by an index α, we have

$$\inf_F Q(F) \geq \inf_{\{n_\alpha\}} \sum_\alpha \inf_{F_\alpha} Q_\alpha(F_\alpha), \tag{6.30}$$

where Q_α is defined by the same formula as Q but with the integrations limited to the box α, F_α is a wave function with particle number n_α, and the infimum is taken over all distributions of the particles with $\sum n_\alpha = N$.

We now fix some $M > 0$, that will eventually tend to ∞, and restrict ourselves to boxes inside a cube Λ_M of side length M. Since $v \geq 0$ the contribution to (6.30) of boxes outside this cube is easily estimated from below by $-8\pi N a \sup_{\vec{x} \notin \Lambda_M} \rho^{\mathrm{GP}}(\vec{x})$, which, divided by N, is arbitrarily small for M large, since Na is fixed and $\phi^{\mathrm{GP}}/N^{1/2} = \phi^{\mathrm{GP}}_{1,Na}$ decreases faster than exponentially at infinity ([LSeY1], Lemma A.5).

For the boxes inside the cube Λ_M we want to use Lemma 2.5 and therefore we must approximate ρ^{GP} by constants in each box. Let $\rho_{\alpha,\max}$ and $\rho_{\alpha,\min}$, respectively, denote the maximal and minimal values of ρ^{GP} in box α. Define

$$\Psi_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) = F_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha})\prod_{k=1}^{n_\alpha}\phi^{\mathrm{GP}}(\vec{x}_k), \tag{6.31}$$

and

$$\Psi_\alpha^{(i)}(\vec{x}_1,\dots,\vec{x}_{n_\alpha}) = F_\alpha(\vec{x}_1,\dots,\vec{x}_{n_\alpha})\prod_{\substack{k=1\\k\neq i}}^{n_\alpha}\phi^{\mathrm{GP}}(\vec{x}_k). \tag{6.32}$$

We have, for all $1 \le i \le n_\alpha$,

$$\begin{aligned}&\int\prod_{k=1}^{n_\alpha}\rho^{\mathrm{GP}}(\vec{x}_k)\left(|\nabla_i F_\alpha|^2 + \tfrac{1}{2}\sum_{j\neq i} v(|\vec{x}_i-\vec{x}_j|)|F_\alpha|^2\right)\\ &\ge \rho_{\alpha,\min}\int\left(|\nabla_i\Psi_\alpha^{(i)}|^2 + \tfrac{1}{2}\sum_{j\neq i} v(|\vec{x}_i-\vec{x}_j|)|\Psi_\alpha^{(i)}|^2\right).\end{aligned} \tag{6.33}$$

We now use Lemma 2.5 to get, for all $0 \le \varepsilon \le 1$,

$$(6.33) \ge \rho_{\alpha,\min}\int\left(\varepsilon|\nabla_i\Psi_\alpha^{(i)}|^2 + a(1-\varepsilon)U(t_i)|\Psi_\alpha^{(i)}|^2\right) \tag{6.34}$$

where t_i is the distance to the nearest neighbor of $\vec{x}_i$, c.f., (2.29), and U the potential (2.30).

Since $\Psi_\alpha = \phi^{\mathrm{GP}}(\vec{x}_i)\Psi_\alpha^{(i)}$ we can estimate

$$|\nabla_i\Psi_\alpha|^2 \le 2\rho_{\alpha,\max}|\nabla_i\Psi_\alpha^{(i)}|^2 + 2|\Psi_\alpha^{(i)}|^2 N C_M \tag{6.35}$$

with

$$C_M = \frac{1}{N}\sup_{\vec{x}\in\Lambda_M}|\nabla\phi^{\mathrm{GP}}(\vec{x})|^2 = \sup_{\vec{x}\in\Lambda_M}|\nabla\phi^{\mathrm{GP}}_{1,Na}(\vec{x})|^2. \tag{6.36}$$

Since Na is fixed, C_M is independent of N. Inserting (6.35) into (6.34), summing over i and using $\rho^{\mathrm{GP}}(\vec{x}_i) \le \rho_{\alpha,\max}$ in the last term of (6.28) (in the box α), we get

$$Q_\alpha(F_\alpha) \ge \frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}}E_\varepsilon^U(n_\alpha, L) - 8\pi a\rho_{\alpha,\max}n_\alpha - \varepsilon C_M n_\alpha, \tag{6.37}$$

where L is the side length of the box and $E_\varepsilon^U(n_\alpha, L)$ is the ground state energy of

$$\sum_{i=1}^{n_\alpha}(-\tfrac{1}{2}\varepsilon\Delta_i + (1-\varepsilon)aU(t_i)) \tag{6.38}$$

in the box (c.f. (2.35)). We want to minimize (6.37) with respect to n_α and drop the subsidiary condition $\sum_\alpha n_\alpha = N$ in (6.30). This can only lower the minimum. For the time being we also ignore the last term in (6.37). (The total contribution of this term for all boxes is bounded by $\varepsilon C_M N$ and will be shown to be negligible compared to the other terms.)

Since the lower bound for the energy of Theorem 2.4 was obtained precisely from a lower bound to the operator (6.38), we can use the statement and proof of Theorem 2.4. From this we see that

$$E_\varepsilon^U(n_\alpha, L) \geq (1-\varepsilon)\frac{4\pi a n_\alpha^2}{L^3}(1 - CY_\alpha^{1/17}) \tag{6.39}$$

with $Y_\alpha = a^3 n_\alpha / L^3$, provided Y_α is small enough, $\varepsilon \geq Y_\alpha^{1/17}$ and $n_\alpha \geq (\text{const.}) Y_\alpha^{-1/17}$. The condition on ε is certainly fulfilled if we choose $\varepsilon = Y^{1/17}$ with $Y = a^3 N / L^3$. We now want to show that the n_α minimizing the right side of (6.37) is large enough for (6.39) to apply.

If the minimum of the right side of (6.37) (without the last term) is taken for some $\bar{n}_\alpha$, we have

$$\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \left(E_\varepsilon^U(\bar{n}_\alpha + 1, L) - E_\varepsilon^U(\bar{n}_\alpha, L)\right) \geq 8\pi a \rho_{\alpha,\max}. \tag{6.40}$$

On the other hand, we claim that

Lemma 6.4. *For any n*

$$E_\varepsilon^U(n+1, L) - E_\varepsilon^U(n, L) \leq 8\pi a \frac{n}{L^3}. \tag{6.41}$$

Proof. Denote the operator (6.38) by $\tilde{H}_n$, with $n_\alpha = n$, and let $\tilde{\Psi}_n$ be its ground state. Let t_i' be the distance to the nearest neighbor of $\vec{x}_i$ among the $n+1$ points $\vec{x}_1, \ldots, \vec{x}_{n+1}$ (without $\vec{x}_i$) and t_i the corresponding distance excluding $\vec{x}_{n+1}$. Obviously, for $1 \leq i \leq n$,

$$U(t_i') \leq U(t_i) + U(|\vec{x}_i - \vec{x}_{n+1}|) \tag{6.42}$$

and

$$U(t_{n+1}') \leq \sum_{i=1}^{n} U(|\vec{x}_i - \vec{x}_{n+1}|). \tag{6.43}$$

Therefore

$$\tilde{H}_{n+1} \leq \tilde{H}_n - \tfrac{1}{2}\varepsilon\Delta_{n+1} + 2a\sum_{i=1}^{n} U(|\vec{x}_i - \vec{x}_{n+1}|). \tag{6.44}$$

Using $\tilde{\Psi}_n / L^{3/2}$ as trial function for $\tilde{H}_{n+1}$ we arrive at (6.41). ∎

Eq. (6.41) together with (6.40) shows that $\bar{n}_\alpha$ is at least $\sim \rho_{\alpha,\max} L^3$. We shall choose $L \sim N^{-1/10}$, so the conditions needed for (6.39) are fulfilled for N large enough, since $\rho_{\alpha,\max} \sim N$ and hence $\bar{n}_\alpha \sim N^{7/10}$ and $Y_\alpha \sim N^{-2}$.

In order to obtain a lower bound on Q_α we therefore have to minimize

$$4\pi a \left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}} \frac{n_\alpha^2}{L^3}\left(1 - CY^{1/17}\right) - 2n_\alpha \rho_{\alpha,\max}\right). \tag{6.45}$$

We can drop the requirement that n_α has to be an integer. The minimum of (6.45) is obtained for

$$n_\alpha = \frac{\rho_{\alpha,\max}^2}{\rho_{\alpha,\min}} \frac{L^3}{(1 - CY^{1/17})}. \tag{6.46}$$

By Eq. (6.27) this gives the following lower bound, including now the last term in (6.37) as well as the contributions from the boxes outside Λ_M,

$$E_0(N,a) - E^{\mathrm{GP}}(N,a) \geq$$
$$4\pi a \int |\rho^{\mathrm{GP}}|^2 - 4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \left(\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \right) \tag{6.47}$$
$$- Y^{1/17} N C_M - 4\pi a N \sup_{\vec{x} \notin \Lambda_M} \rho^{\mathrm{GP}}(\vec{x}).$$

Now ρ^{GP} is differentiable and strictly positive. Since all the boxes are in the fixed cube Λ_M there are constants $C' < \infty$, $C'' > 0$, such that

$$\rho_{\alpha,\max} - \rho_{\alpha,\min} \leq NC'L, \quad \rho_{\alpha,\min} \geq NC''. \tag{6.48}$$

Since $L \sim N^{-1/10}$ and $Y \sim N^{-17/10}$ we therefore have, for large N,

$$\frac{\rho_{\alpha,\max}^3}{\rho_{\alpha,\min}^3} \frac{1}{(1 - CY^{1/17})} \leq 1 + (\text{const.}) N^{-1/10} \tag{6.49}$$

Also,

$$4\pi a \sum_{\alpha \subset \Lambda_M} \rho_{\alpha,\min}^2 L^3 \leq 4\pi a \int |\rho^{\mathrm{GP}}|^2 \leq E^{\mathrm{GP}}(N,a). \tag{6.50}$$

Hence, noting that $E^{\mathrm{GP}}(N,a) = NE^{\mathrm{GP}}(1,Na) \sim N$ since Na is fixed,

$$\frac{E_0(N,a)}{E^{\mathrm{GP}}(N,a)} \geq 1 - (\text{const.})(1 + C_M) N^{-1/10} - (\text{const.}) \sup_{\vec{x} \notin \Lambda_M} |\phi_{1,Na}^{\mathrm{GP}}|^2, \tag{6.51}$$

where the constants depend on Na. We can now take $N \to \infty$ and then $M \to \infty$.

Part 3: Lower bound to the QM energy, TF case. In the above proof of the lower bound in the GP case we did not attempt to keep track of the dependence of the constants on Na. In the TF case $Na \to \infty$, so one would need to take a closer look at this dependence if one wanted to carry the proof directly over to this case. But we don't have to do so, because there is a simpler direct proof. Using the explicit form of the TF minimizer, namely

$$\rho_{N,a}^{\mathrm{TF}}(\vec{x}) = \frac{1}{8\pi a} [\mu^{\mathrm{TF}} - V(\vec{x})]_+, \tag{6.52}$$

where $[t]_+ \equiv \max\{t, 0\}$ and μ^{TF} is chosen so that the normalization condition $\int \rho_{N,a}^{\mathrm{TF}} = N$ holds, we can use

$$V(\vec{x}) \geq \mu^{\mathrm{TF}} - 8\pi a \rho^{\mathrm{TF}}(\vec{x}) \tag{6.53}$$

to get a replacement as in (6.29), but without changing the measure. Moreover, ρ^{TF} has compact support, so, applying again the box method described above, the boxes far out do not contribute to the energy. However, μ^{TF} (which depends only on the combination Na) tends to infinity as $Na \to \infty$. We need to control the asymptotic behavior of μ^{TF}, and this leads to the

restrictions on V described in the paragraph preceding Theorem 6.3. For simplicity, we shall here only consider the case when V itself is homogeneous, i.e., $V(\lambda\vec{x}) = \lambda^s V(\vec{x})$ for all $\lambda > 0$ with some $s > 0$.

In the same way as in (6.6) we have, with $g = Na$,

$$\mu^{\mathrm{TF}}(g) = dE^{\mathrm{TF}}(N,a)/dN = E^{\mathrm{TF}}(1,g) + 4\pi g \int |\rho^{\mathrm{TF}}_{1,g}(\vec{x})|^2 d\vec{x}. \tag{6.54}$$

The TF energy, chemical potential and minimizer satisfy the scaling relations

$$E^{\mathrm{TF}}(1,g) = g^{s/(s+3)} E^{\mathrm{TF}}(1,1), \tag{6.55}$$

$$\mu^{\mathrm{TF}}(g) = g^{s/(s+3)} \mu^{\mathrm{TF}}(1), \tag{6.56}$$

and

$$g^{3/(s+3)} \rho^{\mathrm{TF}}_{1,g}(g^{1/(s+3)}\vec{x}) = \rho^{\mathrm{TF}}_{1,g}(\vec{x}). \tag{6.57}$$

We also introduce the scaled interaction potential, $\widehat{v}$, by

$$\widehat{v}(\vec{x}) = g^{2/(s+3)} v(g^{1/(s+3)}\vec{x}) \tag{6.58}$$

with scattering length

$$\widehat{a} = g^{-1/(s+3)} a. \tag{6.59}$$

Using (6.53), (6.54) and the scaling relations we obtain

$$E_0(N,a) \geq E^{\mathrm{TF}}(N,a) + 4\pi N g^{s/(s+3)} \int |\rho^{\mathrm{TF}}_{1,1}|^2 + g^{-2/(s+3)} Q \tag{6.60}$$

with

$$Q = \inf_{\int |\Psi|^2 = 1} \sum_i \int \left(|\nabla_i \Psi|^2 + \tfrac{1}{2} \sum_{j \neq i} \widehat{v}(\vec{x}_i - \vec{x}_j) |\Psi|^2 - 8\pi N \widehat{a} \rho^{\mathrm{TF}}_{1,1}(\vec{x}_i) |\Psi|^2 \right). \tag{6.61}$$

We can now proceed exactly as in Part 2 to arrive at the analogy of Eq. (6.47), which in the present case becomes

$$E_0(N,a) - E^{\mathrm{TF}}(N,a) \geq$$
$$4\pi N g^{s/(s+3)} \int |\rho^{\mathrm{TF}}_{1,1}|^2 - 4\pi N \widehat{a} \sum_\alpha \rho^2_{\alpha,\max} L^3 (1 - C\widehat{Y}^{1/17})^{-1}. \tag{6.62}$$

Here $\rho_{\alpha,\max}$ is the maximum of $\rho^{\mathrm{TF}}_{1,1}$ in the box α, and $\widehat{Y} = \widehat{a}^3 N/L^3$. This holds as long as L does not decrease too fast with N. In particular, if L is simply fixed, this holds for all large enough N. Note that

$$\bar{\rho} = N\bar{\rho}_{1,g} \sim N g^{-3/(s+3)} \bar{\rho}_{1,1}, \tag{6.63}$$

so that $\widehat{a}^3 N \sim a^3 \bar{\rho}$ goes to zero as $N \to \infty$ by assumption. Hence, if we first let $N \to \infty$ (which implies $\widehat{Y} \to 0$) and then take L to zero, we of arrive at the desired result

$$\liminf_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{TF}}(N,a)} \geq 1 \tag{6.64}$$

in the limit $N \to \infty$, $a^3\bar{\rho} \to 0$. Here we used the fact that (because V, and hence ρ^{TF}, is continuous by assumption) the Riemann sum $\sum_\alpha \rho^2_{\alpha,\max} L^3$

converges to $\int |\rho_{1,1}^{\mathrm{TF}}|^2$ as $L \to 0$. Together with the upper bound (6.25) and the fact that $E^{\mathrm{GP}}(N,a)/E^{\mathrm{TF}}(N,a) = E^{\mathrm{GP}}(1,Na)/E^{\mathrm{TF}}(1,Na) \to 1$ as $Na \to \infty$, which holds under our regularity assumption on V (c.f. Lemma 2.3 in [LSeY2]), this proves (6.14) and (6.20).

Part 4: Convergence of the densities. The convergence of the energies implies the convergence of the densities in the usual way by variation of the external potential. We show here the TF case, the GP case goes analogously. Set again $g = Na$. Making the replacement

$$V(\vec{x}) \longrightarrow V(\vec{x}) + \delta g^{s/(s+3)} Z(g^{-1/(s+3)}\vec{x}) \tag{6.65}$$

for some positive $Z \in C_0^\infty$ and redoing the upper and lower bounds we see that (6.20) holds with W replaced by $W + \delta Z$. Differentiating with respect to δ at $\delta = 0$ yields

$$\lim_{N\to\infty} \frac{g^{3/(s+3)}}{N} \rho_{N,a}^{\mathrm{QM}}(g^{1/(s+3)}\vec{x}) = \tilde{\rho}_{1,1}^{\mathrm{TF}}(\vec{x}) \tag{6.66}$$

in the sense of distributions. Since the functions all have L^1-norm 1, we can conclude that there is even weak L^1-convergence. ∎

6.2. **Two Dimensions.** In contrast to the three-dimensional case the energy per particle for a dilute gas in two dimensions is *nonlinear* in ρ. In view of Schick's formula (3.1) for the energy of the homogeneous gas it would appear natural to take the interaction into account in two dimensional GP theory by a term

$$4\pi \int_{\mathbb{R}^2} |\ln(|\phi(\vec{x})|^2 a^2)|^{-1} |\phi(\vec{x})|^4 d\vec{x}, \tag{6.67}$$

and such a term has, indeed, been suggested in [Sh] and [KNSQ]. However, since the nonlinearity appears only in a logarithm, this term is unnecessarily complicated as far as leading order computations are concerned. For dilute gases it turns out to be sufficient, to leading order, to use an interaction term of the same form as in the three-dimensional case, i.e, define the GP functional as (for simplicity we put $\mu = 1$ in this section)

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \int_{\mathbb{R}^2} \left(|\nabla\phi|^2 + V|\phi|^2 + 4\pi\alpha|\phi|^4 \right) d\vec{x}, \tag{6.68}$$

where instead of a the coupling constant is now

$$\alpha = |\ln(\bar{\rho}_N a^2)|^{-1} \tag{6.69}$$

with $\bar{\rho}_N$ the *mean density* for the GP functional at coupling constant 1 and particle number N. This is defined analogously to (6.12) as

$$\bar{\rho}_N = \frac{1}{N} \int |\phi_{N,1}^{\mathrm{GP}}|^4 d\vec{x} \tag{6.70}$$

where $\phi_{N,1}^{\mathrm{GP}}$ is the minimizer of (6.68) with $\alpha = 1$ and subsidiary condition $\int |\phi|^2 = N$. Note that α in (6.69) depends on N through the mean density.

Let us denote the GP energy for a given N and coupling constant α by $E^{\mathrm{GP}}(N,\alpha)$ and the corresponding minimizer by $\phi^{\mathrm{GP}}_{N,\alpha}$. As in three dimensions the scaling relations

$$E^{\mathrm{GP}}(N,\alpha) = NE^{\mathrm{GP}}(1,N\alpha) \tag{6.71}$$

and

$$N^{-1/2}\phi^{\mathrm{GP}}_{N,\alpha} = \phi^{\mathrm{GP}}_{1,N\alpha}, \tag{6.72}$$

hold, and the relevant parameter is

$$g \equiv N\alpha. \tag{6.73}$$

In three dimensions, where $\alpha = a$, it is natural to consider the limit $N \to \infty$ with $g = Na =$ const. The analogue of Theorem 6.1 in two dimensions is

Theorem 6.5 (Two-dimensional GP limit theorem). *If, for $N \to \infty$, $a^2\bar{\rho}_N \to 0$ with $g = N/|\ln(a^2\bar{\rho}_N)|$ fixed, then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{E^{\mathrm{GP}}(N,1/|\ln(a^2\bar{\rho}_N)|)} = 1 \tag{6.74}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\mathrm{QM}}_{N,a}(\vec{x}) = \left|\phi^{\mathrm{GP}}_{1,g}(\vec{x})\right|^2 \tag{6.75}$$

in the weak L^1-sense.

This result, however, is of rather limited use in practice. The reason is that in two dimensions the scattering length has to decrease exponentially with N if g is fixed. The parameter g is typically *very large* in two dimensions so it is more appropriate to consider the limit $N \to \infty$ and $g \to \infty$ (but still $\bar{\rho}_N a^2 \to 0$).

For potentials V that are *homogeneous* functions of $\vec{x}$, i.e.,

$$V(\lambda\vec{x}) = \lambda^s V(\vec{x}) \tag{6.76}$$

for some $s > 0$, this limit can be described by the a 'Thomas-Fermi' energy functional like (6.19) with coupling constant unity:

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{\mathbb{R}^2} \left(V(\vec{x})\rho(\vec{x}) + 4\pi\rho(\vec{x})^2\right) d\vec{x}. \tag{6.77}$$

This is just the GP functional without the gradient term and $\alpha = 1$. Here ρ is a nonnegative function on $\mathbb{R}^2$ and the normalization condition is

$$\int \rho(\vec{x})d\vec{x} = 1. \tag{6.78}$$

The minimizer of (6.77) can be given explicitly. It is

$$\rho^{\mathrm{TF}}_{1,1}(\vec{x}) = (8\pi)^{-1}[\mu^{\mathrm{TF}} - V(\vec{x})]_+ \tag{6.79}$$

where the chemical potential μ^{TF} is determined by the normalization condition (6.78) and $[t]_+ = t$ for $t \geq 0$ and zero otherwise. We denote the corresponding energy by $E^{\mathrm{TF}}(1,1)$. By scaling one obtains

$$\lim_{g\to\infty} E^{\mathrm{GP}}(1,g)/g^{s/(s+2)} = E^{\mathrm{TF}}(1,1), \tag{6.80}$$

$$\lim_{g\to\infty} g^{2/(s+2)}\rho^{\mathrm{GP}}_{1,g}(g^{1/(s+2)}\vec{x}) = \rho^{\mathrm{TF}}_{1,1}(\vec{x}), \tag{6.81}$$

with the latter limit in the strong L^2 sense.

Our main result about two-dimensional Bose gases in external potentials satisfying (6.76) is that analogous limits also hold for the many-particle quantum mechanical ground state at low densities:

Theorem 6.6 (Two-dimensional TF limit theorem). *In two dimensions, if $a^2\bar{\rho}_N \to 0$, but $g = N/|\ln(\bar{\rho}_N a^2)| \to \infty$ as $N \to \infty$ then*

$$\lim_{N\to\infty} \frac{E_0(N,a)}{g^{s/s+2}} = E^{\mathrm{TF}}(1,1) \tag{6.82}$$

and, in the weak L^1 sense,

$$\lim_{N\to\infty} \frac{g^{2/(s+2)}}{N}\rho^{\mathrm{QM}}_{N,a}(g^{1/(s+2)}\vec{x}) = \rho^{\mathrm{TF}}_{1,1}(\vec{x}). \tag{6.83}$$

Remarks: 1. As in Theorem 6.3, it is sufficient that V is asymptotically equal to some homogeneous potential, W. In this case, $E^{\mathrm{TF}}(1,1)$ and $\rho^{\mathrm{TF}}_{1,1}$ in Theorem 6.6 should be replaced by the corresponding quantities for W.

2. From Eq. (6.81) it follows that

$$\bar{\rho}_N \sim N^{s/(s+2)} \tag{6.84}$$

for large N. Hence the low density criterion $a^2\bar{\rho} \ll 1$, means that $a/L_{\mathrm{osc}} \ll N^{-s/2(s+2)}$.

We shall now comment briefly on the proofs of Theorems 6.5 and 6.6, mainly pointing out the differences from the 3D case considered previously.

The upper bounds for the energy are obtained exactly in a same way as in three dimensions. For the lower bound in Theorem 6.5 the point to notice is that the expression (6.45), that has to be minimized over n_α, is in 2D replaced by

$$4\pi\left(\frac{\rho_{\alpha,\min}}{\rho_{\alpha,\max}}\frac{n_\alpha^2}{L^2}\frac{1}{|\ln(a^2 n_\alpha/L^2)|}\left(1-\frac{C}{|\ln(a^2N/L^2)|^{1/5}}\right) - \frac{2n_\alpha\rho_{\alpha,\max}}{|\ln(a^2\bar{\rho}_N)|}\right), \tag{6.85}$$

since Eq. (6.39) has to be replaced by the analogous inequality for 2D (c.f. (3.31)). To minimize (6.85) we use the following lemma:

Lemma 6.7. *For $0 < x, b < 1$ and $k \geq 1$ we have*

$$\frac{x^2}{|\ln x|} - 2\frac{b}{|\ln b|}xk \geq -\frac{b^2}{|\ln b|}\left(1+\frac{1}{(2|\ln b|)^2}\right)k^2. \tag{6.86}$$

Proof. Replacing x by xk and using the monotonicity of ln we see that it suffices to consider $k = 1$. Since $\ln x \geq -\frac{1}{de}x^{-d}$ for all $d > 0$ we have

$$\frac{x^2}{b^2}\frac{|\ln b|}{|\ln x|} - 2\frac{x}{b} \geq \frac{|\ln b|}{b^2}edx^{2+d} - \frac{2x}{b} \geq c(d)(b^d ed\,|\ln b|)^{-1/(1+d)} \tag{6.87}$$

with

$$c(d) = 2^{(2+d)/(1+d)} \left(\frac{1}{(2+d)^{(2+d)/(1+d)}} - \frac{1}{(2+d)^{1/(1+d)}} \right) \geq -1 - \frac{1}{4}d^2. \tag{6.88}$$

Choosing $d = 1/|\ln b|$ gives the desired result. ∎

Applying this lemma with $x = a^2 n_\alpha / L^2$, $b = a^2 \rho_{\alpha,\max}$ and

$$k = \frac{\rho_{\alpha,\max}}{\rho_{\alpha,\min}} \left(1 - \frac{C}{|\ln(a^2 N/L^2)|^{1/5}} \right)^{-1} \frac{|\ln(a^2 \rho_{\alpha,\max})|}{|\ln(a^2 \bar{\rho}_N)|} \tag{6.89}$$

we get the bound

$$(6.85) \geq -4\pi \frac{\rho_{\alpha,\max}^2 L^2}{|\ln(a^2 \bar{\rho}_N)|} \left(1 + \frac{1}{4|\ln(a^2 \rho_{\alpha,\max})|^2} \right) k. \tag{6.90}$$

In the limit considered, k and the factor in parenthesis both tend to 1 and the Riemann sum over the boxes α converges to the integral as $L \to 0$.

The TF case, Thm. 6.6, is treated in the same way as in three dimensions, with modifications analogous to those just discussed when passing from 3D to 2D in GP theory.

7. Bose-Einstein Condensation and Superfluidity for Dilute Trapped Gases

It was shown in the previous section that, for each fixed Na, the minimization of the GP functional correctly reproduces the large N asymptotics of the ground state energy and density of H – but no assertion about BEC in this limit was made. We will now extend this result by showing that in the Gross-Pitaevskii limit there is indeed 100% Bose condensation in the ground state. This is a generalization of the homogeneous case considered in Theorem 5.1 and although it is not the same as BEC in the thermodynamic limit it is quite relevant for the actual experiments with Bose gases in traps. In the following, we concentrate on the 3D case, but analogous considerations apply also to the 2D case. We also discuss briefly some extensions of Theorem 5.3 pertaining to superfluidity in trapped gases.

As in the last section we choose to keep the length scale L_{osc} of the confining potential fixed and thus write Na instead of Na/L_{osc}. Consequently the powers of N appearing in the proofs are different from those in the proof Theorem 5.1, where we kept Na/L *and* N/L^3 fixed.

For use later, we define the projector

$$P^{\text{GP}} = |\phi^{\text{GP}}\rangle\langle\phi^{\text{GP}}| \,. \tag{7.1}$$

Here (and everywhere else in this section) we denote $\phi^{\text{GP}} \equiv \phi^{\text{GP}}_{1,Na}$ for simplicity, where $\phi^{\text{GP}}_{1,Na}$ is the minimizer of the GP functional (6.2) with parameter Na and normalization condition $\int |\phi|^2 = 1$ (compare with (6.8)). Moreover, we set $\mu \equiv 1$.

In the following, Ψ_0 denotes the (nonnegative and normalized) ground state of the Hamiltonian (6.1). BEC refers to the reduced one-particle density matrix $\gamma(\vec{x},\vec{x}')$ of Ψ_0, defined in (5.1). The precise definition of BEC is is that for some $c > 0$ this integral operator has for all large N an an eigenfunction with eigenvalue $\geq cN$.

Complete (or 100%) BEC is defined to be the property that $\frac{1}{N}\gamma(\vec{x},\vec{x}')$ not only has an eigenvalue of order one, as in the general case of an incomplete BEC, but in the limit it has only one nonzero eigenvalue (namely 1). Thus, $\frac{1}{N}\gamma(\vec{x},\vec{x}')$ becomes a simple product $\varphi(\vec{x})^*\varphi(\vec{x}')$ as $N \to \infty$, in which case φ is called the *condensate wave function.* In the GP limit, i.e., $N \to \infty$ with Na fixed, we can show that this is the case, and the condensate wave function is, in fact, the GP minimizer ϕ^{GP}.

Theorem 7.1 (Bose-Einstein condensation in a trap). *For each fixed* Na

$$\lim_{N\to\infty} \frac{1}{N}\gamma(\vec{x},\vec{x}') = \phi^{\mathrm{GP}}(\vec{x})\phi^{\mathrm{GP}}(\vec{x}') \ .$$

in trace norm, i.e., $\mathrm{Tr}\,\left|\frac{1}{N}\gamma - P^{\mathrm{GP}}\right| \to 0$.

We remark that Theorem 7.1 implies that there is also 100% condensation for all n-particle reduced density matrices

$$\begin{aligned}&\gamma^{(n)}(\vec{x}_1,\dots,\vec{x}_n;\vec{x}_1',\dots,\vec{x}_n')\\ &= n!\binom{N}{n}\int \Psi_0(\vec{x}_1,\dots,\vec{x}_N)\Psi_0(\vec{x}_1',\dots,\vec{x}_n',\vec{x}_{n+1},\dots\vec{x}_N)d\vec{x}_{n+1}\cdots d\vec{x}_N\end{aligned} \tag{7.2}$$

of Ψ_0, i.e., they converge, after division by the normalization factor, to the one-dimensional projector onto the n-fold tensor product of ϕ^{GP}. In other words, for n fixed particles the probability of finding them all in the same state ϕ^{GP} tends to 1 in the limit considered. To see this, let a^*, a denote the boson creation and annihilation operators for the state ϕ^{GP}, and observe that

$$1 \geq \lim_{N\to\infty} N^{-n}\langle\Psi_0|(a^*)^n a^n|\Psi_0\rangle = \lim_{N\to\infty} N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle \ , \tag{7.3}$$

since the terms coming from the commutators $[a,a^*] = 1$ are of lower order as $N \to \infty$ and vanish in the limit. From convexity it follows that

$$N^{-n}\langle\Psi_0|(a^*a)^n|\Psi_0\rangle \geq N^{-n}\langle\Psi_0|a^*a|\Psi_0\rangle^n \tag{7.4}$$

which converges to 1 as $N \to \infty$, proving our claim.

Another corollary, important for the interpretation of experiments, concerns the momentum distribution of the ground state.

Corollary 7.2 (Convergence of momentum distribution). *Let*

$$\widehat{\rho}(\vec{k}) = \int\int \gamma(\vec{x},\vec{x}')\exp[i\vec{k}\cdot(\vec{x}-\vec{x}')]d\vec{x}d\vec{x}'$$

denote the one-particle momentum density of Ψ_0. *Then, for fixed* Na,

$$\lim_{N\to\infty} \frac{1}{N}\widehat{\rho}(\vec{k}) = |\widehat{\phi}^{\mathrm{GP}}(\vec{k})|^2$$

strongly in $L^1(\mathbb{R}^3)$. *Here,* $\widehat{\phi}^{\mathrm{GP}}$ *denotes the Fourier transform of* ϕ^{GP}.

Proof. If $\mathcal{F}$ denotes the (unitary) operator 'Fourier transform' and if h is an arbitrary L^∞-function, then

$$\begin{aligned}\left|\frac{1}{N}\int \widehat{\rho}h - \int |\widehat{\phi}^{\mathrm{GP}}|^2 h\right| &= \left|\mathrm{Tr}\,[\mathcal{F}^{-1}(\gamma/N - P^{\mathrm{GP}})\mathcal{F}h]\right| \\ &\leq \|h\|_\infty \mathrm{Tr}\,|\gamma/N - P^{\mathrm{GP}}|,\end{aligned}$$

from which we conclude that

$$\|\widehat{\rho}/N - |\widehat{\phi}^{\mathrm{GP}}|^2\|_1 \leq \mathrm{Tr}\,|\gamma/N - P^{\mathrm{GP}}|\,.$$

■

As already stated, Theorem 7.1 is a generalization of Theorem 5.1, the latter corresponding to the case that V is a box potential. It should be noted, however, that we use different scaling conventions in these two theorems: In Theorem 5.1 the box size grows as $N^{1/3}$ to keep the density fixed, while in Theorem 7.1 we choose to keep the confining external potential fixed. Both conventions are equivalent, of course, c.f. the remarks in the second paragraph of Section 6, but when comparing the exponents of N that appear in the proofs of the two theorems the different conventions should be born in mind.

As in Theorem 5.1 there are two essential components of our proof of Theorem 7.1. The first is a proof that the part of the kinetic energy that is associated with the interaction v (namely, the second term in (6.16a)) is mostly located in small balls surrounding each particle. More precisely, these balls can be taken to have radius roughly $N^{-5/9}$, which is much smaller than the mean-particle spacing $N^{-1/3}$. (The exponents differ from those of Lemma 5.2 because of different scaling conventions.) This allows us to conclude that the function of $\vec{x}$ defined for each fixed value of $\vec{X}$ by

$$f_{\vec{X}}(\vec{x}) = \frac{1}{\phi^{\mathrm{GP}}(\vec{x})}\Psi_0(\vec{x},\vec{X}) \geq 0 \tag{7.5}$$

has the property that $\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})$ is almost zero outside the small balls centered at points of $\vec{X}$.

The complement of the small balls has a large volume but it can be a weird set; it need not even be connected. Therefore, the smallness of $\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})$ in this set does not guarantee that $f_{\vec{X}}(\vec{x})$ is nearly constant (in $\vec{x}$), or even that it is continuous. We need $f_{\vec{X}}(\vec{x})$ to be nearly constant in order to conclude BEC. What saves the day is the knowledge that the total kinetic energy of $f_{\vec{X}}(\vec{x})$ (including the balls) is not huge. The result that allows us to combine these two pieces of information in order to deduce the almost constancy of

$f_{\vec{X}}(\vec{x})$ is the generalized Poincaré inequality in Lemma 4.3. The important point in this lemma is that there is no restriction on Ω concerning regularity or connectivity.

Using the results of Theorem 6.2, partial integration and the GP equation (i.e., the variational equation for ϕ^{GP}, see Eq. (6.5)) we see that

$$\lim_{N\to\infty} \int |\phi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x}\, d\vec{X} = 4\pi N a s \int |\phi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x}\,. \tag{7.6}$$

The following Lemma shows that to leading order all the energy in (7.6) is concentrated in small balls.

Lemma 7.3 (Localization of the energy in a trap). *For fixed $\vec{X}$ let*

$$\Omega_{\vec{X}} = \left\{ \vec{x} \in \mathbb{R}^3 \,\middle|\, \min_{k\geq 2} |\vec{x} - \vec{x}_k| \geq N^{-1/3-\delta} \right\} \tag{7.7}$$

for some $0 < \delta < 2/9$. Then

$$\lim_{N\to\infty} \int d\vec{X} \int_{\Omega_{\vec{X}}} d\vec{x} |\phi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 = 0\,.$$

Remark. In the proof of Theorem 5.1 we chose δ to be $4/51$, but the following proof shows that one can extend the range of δ beyond this value.

Proof. We shall show that

$$\begin{aligned} &\int d\vec{X} \int_{\Omega^c_{\vec{X}}} d\vec{x} |\phi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 \\ &+ \int d\vec{X} \int d\vec{x} |\phi^{\mathrm{GP}}(\vec{x})|^2 |f_{\vec{X}}(\vec{x})|^2 \left[\tfrac{1}{2} \sum_{k\geq 2} v(|\vec{x} - \vec{x}_k|) - 8\pi N a |\phi^{\mathrm{GP}}(\vec{x})|^2 \right] \\ &\geq -4\pi N a \int |\phi^{\mathrm{GP}}(\vec{x})|^4 d\vec{x} - o(1) \end{aligned} \tag{7.8}$$

as $N \to \infty$. We claim that this implies the assertion of the Lemma. To see this, note that the left side of (7.8) can be written as

$$\frac{1}{N} E_0 - \mu^{\mathrm{GP}} - \int d\vec{X} \int_{\Omega_{\vec{X}}} d\vec{x} |\phi^{\mathrm{GP}}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2\,, \tag{7.9}$$

where we used partial integration and the GP equation (6.5), and also the symmetry of Ψ_0. The convergence of the energy in Theorem 6.1 and the relation (6.6) now imply the desired result.

The proof of (7.8) is actually just a detailed examination of the lower bounds to the energy derived in [LSeY1] and [LY1] and described in Sections 2 and 6. We use the same methods as there, just describing the differences from the case considered here.

Writing

$$f_{\vec{X}}(\vec{x}) = \prod_{k\geq 2} \phi^{\mathrm{GP}}(\vec{x}_k) F(\vec{x}, \vec{X}) \tag{7.10}$$

and using that F is symmetric in the particle coordinates, we see that (7.8) is equivalent to

$$\frac{1}{N}Q_\delta(F) \geq -4\pi Na \int |\phi^{\mathrm{GP}}|^4 - o(1), \tag{7.11}$$

where Q_δ is the quadratic form

$$\begin{aligned} Q_\delta(F) &= \sum_{i=1}^N \int_{\Omega_i^c} |\nabla_i F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\vec{x}_k)|^2 d\vec{x}_k \\ &+ \sum_{1\leq i<j\leq N} \int v(|\vec{x}_i - \vec{x}_j|)|F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\vec{x}_k)|^2 d\vec{x}_k \\ &-8\pi Na \sum_{i=1}^N \int |\phi^{\mathrm{GP}}(\vec{x}_i)|^2 |F|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\vec{x}_k)|^2 d\vec{x}_k. \end{aligned} \tag{7.12}$$

Here Ω_i^c denotes the set

$$\Omega_i^c = \{(\vec{x}_1, \vec{X}) \in \mathbb{R}^{3N} | \min_{k\neq i} |\vec{x}_i - \vec{x}_k| \leq N^{-1/3-\delta}\}.$$

While (7.11) is not true for all conceivable F's satisfying the normalization condition

$$\int |F(\vec{x}, \vec{X})|^2 \prod_{k=1}^N |\phi^{\mathrm{GP}}(\vec{x}_k)|^2 d\vec{x}_k = 1,$$

it *is* true for an F, such as ours, that has bounded kinetic energy (7.6). Looking at Section 6, we see that Eqs. (6.27)–(6.28), (6.47)–(6.51) are similar to (7.11), (7.12) and almost establish (7.11), but there are differences which we now explain.

In our case, the kinetic energy of particle i is restricted to the subset of $\mathbb{R}^{3N}$ in which $\min_{k\neq i} |\vec{x}_i - \vec{x}_k| \leq N^{-1/3-\delta}$. However, looking at the proof of the lower bound to the ground state energy of a homogeneous Bose gas discussed in Section 2, which enters the proof of Theorem 6.1, we see that if we choose $\delta \leq 4/51$ only this part of the kinetic energy is needed for the lower bound, except for some part with a relative magnitude of the order $\varepsilon = O(N^{-2\alpha})$ with $\alpha = 1/17$. (Here we use the a priori knowledge that the kinetic energy is bounded by (7.6).) We can even do better and choose some $4/51 < \delta < 2/9$, if α is chosen small enough. (To be precise, we choose $\beta = 1/3+\alpha$ and $\gamma = 1/3-4\alpha$ in the notation of (2.56), and α small enough). The choice of α only affects the magnitude of the error term, however, which is still $o(1)$ as $N \to \infty$. ∎

Proof of Theorem 7.1. For some $R > 0$ let $\mathcal{K} = \{\vec{x} \in \mathbb{R}^3, |\vec{x}| \leq R\}$, and define

$$\langle f_{\vec{X}} \rangle_{\mathcal{K}} = \frac{1}{\int_{\mathcal{K}} |\phi^{\mathrm{GP}}(\vec{x})|^2 d\vec{x}} \int_{\mathcal{K}} |\phi^{\mathrm{GP}}(\vec{x})|^2 f_{\vec{X}}(\vec{x})\, d\vec{x}\,.$$

We shall use Lemma 4.3, with $d = 3$, $h(\vec{x}) = |\phi^{\rm GP}(\vec{x})|^2 / \int_{\mathcal{K}} |\phi^{\rm GP}|^2$, $\Omega = \Omega_{\vec{X}} \cap \mathcal{K}$ and $f(\vec{x}) = f_{\vec{X}}(\vec{x}) - \langle f_{\vec{X}} \rangle_{\mathcal{K}}$ (see (7.7) and (7.5)). Since $\phi^{\rm GP}$ is bounded on $\mathcal{K}$ above and below by some positive constants, this Lemma also holds (with a different constant C') with $d\vec{x}$ replaced by $|\phi^{\rm GP}(\vec{x})|^2 d\vec{x}$ in (4.4). Therefore,

$$\begin{aligned} &\int d\vec{X} \int_{\mathcal{K}} d\vec{x} |\phi^{\rm GP}(\vec{x})|^2 \left[f_{\vec{X}}(\vec{x}) - \langle f_{\vec{X}} \rangle_{\mathcal{K}} \right]^2 \\ &\leq C' \int d\vec{X} \left[\int_{\Omega_{\vec{X}} \cap \mathcal{K}} |\phi^{\rm GP}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x} \right. \\ &\qquad \left. + \frac{N^{-2\delta}}{R^2} \int_{\mathcal{K}} |\phi^{\rm GP}(\vec{x})|^2 |\nabla_{\vec{x}} f_{\vec{X}}(\vec{x})|^2 d\vec{x} \right], \end{aligned} \tag{7.13}$$

where we used that $|\Omega_{\vec{X}}^c \cap \mathcal{K}| \leq (4\pi/3) N^{-3\delta}$. The first integral on the right side of (7.13) tends to zero as $N \to \infty$ by Lemma 7.3, and the second is bounded by (7.6). We conclude, since

$$\int_{\mathcal{K}} |\phi^{\rm GP}(\vec{x})|^2 f_{\vec{X}}(\vec{x}) d\vec{x} \leq \int_{\mathbb{R}^3} |\phi^{\rm GP}(\vec{x})|^2 f_{\vec{X}}(\vec{x}) d\vec{x}$$

because of the positivity of $f_{\vec{X}}$, that

$$\begin{aligned} \liminf_{N\to\infty} \frac{1}{N} \langle \phi^{\rm GP} | \gamma | \phi^{\rm GP} \rangle &\geq \int_{\mathcal{K}} |\phi^{\rm GP}(\vec{x})|^2 d\vec{x} \lim_{N\to\infty} \int d\vec{X} \int_{\mathcal{K}} d\vec{x} |\Psi_0(\vec{x}, \vec{X})|^2 \\ &= \left[\int_{\mathcal{K}} |\phi^{\rm GP}(\vec{x})|^2 d\vec{x} \right]^2, \end{aligned}$$

where the last equality follows from (6.15). Since the radius of $\mathcal{K}$ was arbitrary, we conclude that

$$\lim_{N\to\infty} \frac{1}{N} \langle \phi^{\rm GP} | \gamma | \phi^{\rm GP} \rangle = 1,$$

implying convergence of γ/N to $P^{\rm GP}$ in Hilbert-Schmidt norm. Since the traces are equal, convergence even holds in trace norm (cf. [Si], Thm. 2.20), and Theorem 7.1 is proven. ∎

We remark that the method presented here also works in the case of a two-dimensional Bose gas. The relevant parameter to be kept fixed in the GP limit is $N/|\ln(a^2 \bar{\rho}_N)|$, all other considerations carry over without essential change, using the results in [LSeY2, LY2], c.f. Sections 3 and 6.2. It should be noted that the existence of BEC in the ground state in 2D is not in conflict with its absence at positive temperatures [Ho, M]. In the hard core lattice gas at half filling precisely this phenomenon occurs [KLS].

of

Finally, we remark on generalizations of Theorem 5.3 on superfluidity from a torus to some physically more realistic settings. As an example, let $\mathcal{C}$ be a finite cylinder based on an annulus centered at the origin. Given a

bounded, real function $a(r,z)$ let A be the vector field (in polar coordinates) $A(r,\theta,z) = \varphi a(r,z)\hat{e}_\theta$, where $\hat{e}_\theta$ is the unit vector in the θ direction. We also allow for a bounded external potential $V(r,z)$ that does not depend on θ.

Using the methods of Appendix A in [LSeY1], it is not difficult to see that there exists a $\varphi_0 > 0$, depending only on $\mathcal{C}$ and $a(r,z)$, such that for all $|\varphi| < \varphi_0$ there is a unique minimizer ϕ^{GP} of the Gross-Pitaevskii functional

$$\mathcal{E}^{\mathrm{GP}}[\phi] = \int_{\mathcal{C}} \Big(\big|\big(\nabla + \mathrm{i}A(\vec{x})\big)\phi(\vec{x})\big|^2 + V(\vec{x})|\phi(\vec{x})|^2 + 4\pi\mu N a|\phi(\vec{x})|^4 \Big) d\vec{x} \quad (7.14)$$

under the normalization condition $\int |\phi|^2 = 1$. This minimizer does not depend on θ, and can be chosen to be positive, for the following reason: The relevant term in the kinetic energy is $T = -r^{-2}[\partial/\partial\theta + \mathrm{i}\varphi r\, a(r,z)]^2$. If $|\varphi r\, a(r,z)| < 1/2$, it is easy to see that $T \geq \varphi^2 a(r,z)^2$, in which case, without raising the energy, we can replace ϕ by the square root of the θ-average of $|\phi|^2$. This can only lower the kinetic energy [LLo] and, by convexity of $x \to x^2$, this also lowers the ϕ^4 term.

We denote the ground state energy of $\mathcal{E}^{\mathrm{GP}}$ by E^{GP}, depending on Na and φ. The following Theorem 7.4 concerns the ground state energy E_0 of

$$H_N^A = \sum_{j=1}^{N} \Big[-\big(\nabla_j + \mathrm{i}A(\vec{x}_j)\big)^2 + V(\vec{x}_j) \Big] + \sum_{1 \leq i < j \leq N} v(|\vec{x}_i - \vec{x}_j|)\,, \quad (7.15)$$

with Neumann boundary conditions on $\mathcal{C}$, and the one-particle reduced density matrix γ_N of the ground state, respectively. Different boundary conditions can be treated in the same manner, if they are also used in (7.14).

Remark. As a special case, consider a uniformly rotating system. In this case $A(\vec{x}) = \varphi r\hat{e}_\theta$, where 2φ is the angular velocity. H_N^A is the Hamiltonian in the rotating frame, but with external potential $V(\vec{x}) + A(\vec{x})^2$ (see e.g. [Bm, p. 131]).

Theorem 7.4 (Superfluidity in a cylinder). *For* $|\varphi| < \varphi_0$

$$\lim_{N\to\infty} \frac{E_0(N,a,\varphi)}{N} = E^{\mathrm{GP}}(Na,\varphi) \quad (7.16)$$

in the limit $N \to \infty$ *with* Na *fixed. In the same limit,*

$$\lim_{N\to\infty} \frac{1}{N}\gamma_N(\vec{x},\vec{x}') = \phi^{\mathrm{GP}}(\vec{x})\phi^{\mathrm{GP}}(\vec{x}') \quad (7.17)$$

in trace class norm, i.e., $\lim_{N\to\infty} \mathrm{Tr}\,\big[\,\big|\gamma_N/N - |\phi^{\mathrm{GP}}\rangle\langle\phi^{\mathrm{GP}}|\,\big|\,\big] = 0$.

In the case of a uniformly rotating system, where 2φ is the angular velocity, the condition $|\varphi| < \varphi_0$ in particular means that the angular velocity is smaller than the critical velocity for creating vortices [Se3, FS].

Remark. In the special case of the curl-free vector potential $A(r,\theta) = \varphi r^{-1}\hat{e}_\theta$, i.e., $a(r,z) = r^{-1}$, one can say more about the role of φ_0. In this case, there is a unique GP minimizer for all $\varphi \notin \mathbb{Z} + \frac{1}{2}$, whereas there

are two minimizers for $\varphi \in \mathbb{Z} + \frac{1}{2}$. Part two of Theorem 7.4 holds in this special case for all $\varphi \notin \mathbb{Z} + \frac{1}{2}$, and (7.16) is true even for all φ.

8. One-Dimensional Behavior of Dilute Bose Gases in Traps

Recently it has become possible to do experiments in highly elongated traps on ultra-cold Bose gases that are effectively one-dimensional [BBD, Go, G, Sc, MSKE]. These experiments show peculiar features predicted by a model of a one-dimensional Bose gas with repulsive δ-function pair interaction, analyzed long ago by Lieb and Liniger [LL]. These include quasi-fermionic behavior [Gi], the absence of Bose-Einstein condensation (BEC) in a dilute limit [Le, PiSt, GWT], and an excitation spectrum different from that predicted by Bogoliubov's theory [LL, JK, KP]. The theoretical work on the dimensional cross-over for the ground state in elongated traps has so far been based either on variational calculations, starting from a 3D delta-potential [Ol, DGW, GW], or on numerical Quantum Monte Carlo studies [Bl, AG] with more realistic, genuine 3D potentials, but particle numbers limited to the order of 100. This work is important and has led to valuable insights, in particular about different parameter regions [PSW, DLO], but a more thorough theoretical understanding is clearly desirable since this is not a simple problem. In fact, it is evident that for a potential with a hard core the true 3D wave functions do not approximately factorize in the longitudinal and transverse variables (otherwise the energy would be infinite) and the effective 1D potential can not be obtained by simply integrating out the transverse variables of the 3D potential (that would immediately create an impenetrable barrier in 1D). It is important to be able to demonstrate rigorously, and therefore unambiguously, that the 1D behavior really follows from the fundamental Schrödinger equation. It is also important to delineate, as we do here, precisely what can be seen in the different parameter regions. The full proofs of our assertions are long and are given in [LSeY6]. Here we state our main results and outline the basic ideas for the proofs.

We start by describing the setting more precisely. It is convenient to write the Hamiltonian in the following way (in units where $\hbar = 2m = 1$):

$$H_{N,L,r,a} = \sum_{j=1}^{N} \left(-\Delta_j + V_r^{\perp}(\vec{x}_j^{\perp}) + V_L(z_j) \right) + \sum_{1 \le i < j \le N} v_a(|\vec{x}_i - \vec{x}_j|) \quad (8.1)$$

with $\vec{x} = (x, y, z) = (\vec{x}^{\perp}, z)$ and with

$$V_r^{\perp}(\vec{x}^{\perp}) = \frac{1}{r^2} V^{\perp}(\vec{x}^{\perp}/r) \,,$$

$$V_L(z) = \frac{1}{L^2} V(z/L) \,, \quad v_a(|\vec{x}|) = \frac{1}{a^2} v(|\vec{x}|/a) \,. \quad (8.2)$$

Here, r, L, a are variable scaling parameters while $V^{\perp}$, V and v are fixed.

We shall be concerned with the ground state of this Hamiltonian for large particle number N, which is appropriate for the consideration of actual experiments. The other parameters of the problem are the scattering length, a, of the two-body interaction potential, v, and two lengths, r and L, describing the transverse and the longitudinal extension of the trap potential, respectively.

The interaction potential v is supposed to be nonnegative, of finite range and have scattering length 1; the scaled potential v_a then has scattering length a. The external trap potentials V and $V^\perp$ confine the motion in the longitudinal (z) and the transversal ($\vec{x}^\perp$) directions, respectively, and are assumed to be continuous and tend to ∞ as $|z|$ and $|\vec{x}^\perp|$ tend to ∞. To simplify the discussion we find it also convenient to assume that V is homogeneous of some order $s > 0$, namely $V(z) = |z|^s$, but weaker assumptions, e.g. asymptotic homogeneity (cf. Section 6), would in fact suffice. The case of a simple box with hard walls is realized by taking $s = \infty$, while the usual harmonic approximation is $s = 2$. It is understood that the lengths associated with the ground states of $-d^2/dz^2 + V(z)$ and $-\Delta^\perp + V^\perp(\vec{x}^\perp)$ are both of the order 1 so that L and r measure, respectively, the longitudinal and the transverse extensions of the trap. We denote the ground state energy of (8.1) by $E^{\mathrm{QM}}(N, L, r, a)$ and the ground state particle density by $\rho^{\mathrm{QM}}_{N,L,r,a}(\vec{x})$. On the average, this 3D density will always be low in the parameter range considered here (in the sense that distance between particles is large compared to the 3D scattering length). The effective 1D density can be either high or low, however.

In parallel with the 3D Hamiltonian we consider the Hamiltonian for n Bosons in 1D with delta interaction and coupling constant $g \geq 0$, i.e.,

$$H^{\mathrm{1D}}_{n,g} = \sum_{j=1}^{n} -\partial^2/\partial z_j^2 + g \sum_{1 \leq i < j \leq n} \delta(z_i - z_j) \ . \tag{8.3}$$

We consider this Hamiltonian for the z_j in an interval of length ℓ in the thermodynamic limit, $\ell \to \infty$, $n \to \infty$ with $\rho = n/\ell$ fixed. The ground state energy per particle in this limit is independent of boundary conditions and can, according to [LL], be written as

$$e^{\mathrm{1D}}_0(\rho) = \rho^2 e(g/\rho) \ , \tag{8.4}$$

with a function $e(t)$ determined by a certain integral equation. Its asymptotic form is $e(t) \approx \frac{1}{2}t$ for $t \ll 1$ and $e(t) \to \pi^2/3$ for $t \to \infty$. Thus

$$e^{\mathrm{1D}}_0(\rho) \approx \tfrac{1}{2} g\rho \quad \text{for} \quad g/\rho \ll 1 \tag{8.5}$$

and

$$e^{\mathrm{1D}}_0(\rho) \approx (\pi^2/3)\rho^2 \quad \text{for} \quad g/\rho \gg 1 \ . \tag{8.6}$$

This latter energy is the same as for non-interacting fermions in 1D, which can be understood from the fact that (8.3) with $g = \infty$ is equivalent to a Hamiltonian describing free fermions.

Taking $\rho e_0^{\mathrm{1D}}(\rho)$ as a local energy density for an inhomogeneous 1D system we can form the energy functional

$$\mathcal{E}[\rho] = \int_{-\infty}^{\infty} \left(|\nabla \sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z)) \right) dz \ . \tag{8.7}$$

Its ground state energy is obtained by minimizing over all normalized densities, i.e.,

$$E^{\mathrm{1D}}(N, L, g) = \inf \left\{ \mathcal{E}[\rho] \ : \ \rho(z) \geq 0, \ \int_{-\infty}^{\infty} \rho(z) dz = N \right\}. \tag{8.8}$$

Using convexity of the map $\rho \mapsto \rho^3 e(g/\rho)$, it is standard to show that there exists a unique minimizer of (8.7) (see, e.g., [LSeY1]). It will be denoted by $\rho_{N,L,g}$. We also define the *mean 1D density* of this minimizer to be

$$\bar{\rho} = \frac{1}{N} \int_{-\infty}^{\infty} (\rho_{N,L,g}(z))^2 \, dz \ . \tag{8.9}$$

In a rigid box, i.e., for $s = \infty$, $\bar{\rho}$ is simply N/L (except for boundary corrections), but in more general traps it depends also on g besides N and L. The order of magnitude of $\bar{\rho}$ in the various parameter regions will be described below.

Our main result relates the 3D ground state energy of (8.1) to the 1D density functional energy $E^{\mathrm{1D}}(N, L, g)$ in the large N limit with $g \sim a/r^2$ provided r/L and a/r are sufficiently small. To state this precisely, let $e^{\perp}$ and $b(\vec{x}^{\perp})$, respectively, denote the ground state energy and the normalized ground state wave function of $-\Delta^{\perp} + V^{\perp}(\vec{x}^{\perp})$. The corresponding quantities for $-\Delta^{\perp} + V_r^{\perp}(\vec{x}^{\perp})$ are $e^{\perp}/r^2$ and $b_r(\vec{x}^{\perp}) = (1/r)b(\vec{x}^{\perp}/r)$. In the case that the trap is a cylinder with hard walls b is a Bessel function; for a quadratic $V^{\perp}$ it is a Gaussian.

Define g by

$$g = \frac{8\pi a}{r^2} \int |b(\vec{x}^{\perp})|^4 d\vec{x}^{\perp} = 8\pi a \int |b_r(\vec{x}^{\perp})|^4 d\vec{x}^{\perp}. \tag{8.10}$$

Our main result of this section is:

Theorem 8.1 (From 3D to 1D). *Let $N \to \infty$ and simultaneously $r/L \to 0$ and $a/r \to 0$ in such a way that $r^2 \bar{\rho} \cdot \min\{\bar{\rho}, g\} \to 0$. Then*

$$\lim \frac{E^{\mathrm{QM}}(N, L, r, a) - N e^{\perp}/r^2}{E^{\mathrm{1D}}(N, L, g)} = 1. \tag{8.11}$$

An analogous result hold for the ground state density. Define the 1D QM density by averaging over the transverse variables, i.e.,

$$\hat{\rho}^{\mathrm{QM}}_{N,L,r,a}(z) \equiv \int \rho^{\mathrm{QM}}_{N,L,r,a}(\vec{x}^{\perp}, z) d\vec{x}^{\perp} \ . \tag{8.12}$$

Let $\bar{L} := N/\bar{\rho}$ denote the extension of the system in z-direction, and define the rescaled density $\widetilde{\rho}$ by

$$\rho^{\mathrm{1D}}_{N,L,g}(z) = \frac{N}{L}\widetilde{\rho}(z/\bar{L}) \,. \tag{8.13}$$

Note that, although $\widetilde{\rho}$ depends on N, L and g, $\|\widetilde{\rho}\|_1 = \|\widetilde{\rho}\|_2 = 1$, which shows in particular that $\bar{L}$ is the relevant scale in z-direction. The result for the ground state density is:

Theorem 8.2 (1D limit for density). *In the same limit as considered in Theorem 8.1,*

$$\lim \left(\frac{\bar{L}}{N} \hat{\rho}^{\mathrm{QM}}_{N,L,r,a}(z\bar{L}) - \widetilde{\rho}(z) \right) = 0 \tag{8.14}$$

in weak L^1 sense.

Note that because of (8.5) and (8.6) the condition $r^2\bar{\rho} \cdot \min\{\bar{\rho}, g\} \to 0$ is the same as

$$e_0^{\mathrm{1D}}(\bar{\rho}) \ll 1/r^2 \,, \tag{8.15}$$

i.e., the average energy per particle associated with the longitudinal motion should be much smaller than the energy gap between the ground and first excited state of the confining Hamiltonian in the transverse directions. Thus, the basic physics is highly quantum-mechanical and has no classical counterpart. The system can be described by a 1D functional (8.7), *even though the transverse trap dimension is much larger than the range of the atomic forces.*

8.1. **Discussion of the results.** We will now give a discussion of the various parameter regions that are included in the limit considered in Theorems 8.1 and 8.2 above. We begin by describing the division of the space of parameters into two basic regions. This decomposition will eventually be refined into five regions, but for the moment let us concentrate on the basic dichotomy.

In Section 6 we proved that the 3D Gross-Pitaevskii formula for the energy is correct to leading order in situations in which N is large but a is small compared to the mean particle distance. This energy has two parts: The energy necessary to confine the particles in the trap, plus the internal energy of interaction, which is $N4\pi a\rho^{\mathrm{3D}}$. This formula was proved to be correct for a *fixed* confining potential in the limit $N \to \infty$ with $a^3\rho^{\mathrm{3D}} \to 0$. However, this limit does not hold uniformly if r/L gets small as N gets large. In other words, new physics can come into play as $r/L \to 0$ and it turns out that this depends on the ratio of a/r^2 to the 1D density, or, in other words, on $g/\bar{\rho}$. There are two basic regimes to consider in highly elongated traps, i.e., when $r \ll L$. They are

- The 1D limit of the 3D Gross-Pitaevskii regime
- The 'true' 1D regime.

The former is characterized by $g/\bar{\rho} \ll 1$, while in the latter regime $g/\bar{\rho}$ is of the order one or even tends to infinity. (If $g/\bar{\rho} \to \infty$ the particles are effectively impenetrable; this is usually referred to as the Girardeau-Tonks region.) These two situations correspond to high 1D density (weak interaction) and low 1D density (strong interaction), respectively. Physically, the main difference is that in the strong interaction regime the motion of the particles in the longitudinal direction is highly correlated, while in the weak interaction regime it is not. Mathematically, this distinction also shows up in our proofs. The first region is correctly described by both the 3D and 1D theories because the two give the same predictions there. That's why we call the second region the 'true' 1D regime.

In both regions the internal energy of the gas is small compared to the energy of confinement. However, this in itself does not imply a specifically 1D behavior. (If a is sufficiently small it is satisfied in a trap of any shape.) 1D behavior, when it occurs, manifests itself by the fact that the transverse motion of the atoms is uncorrelated while the longitudinal motion is correlated (very roughly speaking) in the same way as pearls on a necklace. Thus, the true criterion for 1D behavior is that $g/\bar{\rho}$ is of order unity or larger and not merely the condition that the energy of confinement dominates the internal energy.

We shall now briefly describe the finer division of these two regimes into five regions altogether. Three of them (Regions 1–3) belong to the weak interaction regime and two (Regions 4–5) to the strong interaction regime. They are characterized by the behavior of $g/\bar{\rho}$ as $N \to \infty$. In each of these regions the general functional (8.7) can be replaced by a different, simpler functional, and the energy $E^{1D}(N, L, g)$ in Theorem 8.1 by the ground state energy of that functional. Analogously, the density in Theorem 8.2 can be replaced by the minimizer of the functional corresponding to the region considered.

The five regions are

• **Region 1, the Ideal Gas case:** In the trivial case where the interaction is so weak that it effectively vanishes in the large N limit and everything collapses to the ground state of $-d^2/dz^2 + V(z)$ with ground state energy $e^{\|}$, the energy E^{1D} in (8.11) can be replaced by $Ne^{\|}/L^2$. This is the case if $g/\bar{\rho} \ll N^{-2}$, and the mean density is just $\bar{\rho} \sim N/L$. Note that $g/\bar{\rho} \ll N^{-2}$ means that the 3D interaction energy per particle $\sim a\rho^{3D} \ll 1/L^2$.

• **Region 2, the 1D GP case:** In this region $g/\bar{\rho} \sim N^{-2}$, with $\bar{\rho} \sim N/L$. This case is described by a 1D Gross-Pitaevskii energy functional of the form

$$\mathcal{E}^{GP}[\rho] = \int_{-\infty}^{\infty} \left(|\nabla \sqrt{\rho}(z)|^2 + V_L(z)\rho(z) + \tfrac{1}{2} g \rho(z)^2 \right) dz \,, \tag{8.16}$$

corresponding to the high density approximation (8.5) of the interaction energy in (8.7). Its ground state energy, E^{GP}, fulfills the scaling relation $E^{GP}(N, L, g) = NL^{-2}E^{GP}(1, 1, NgL)$.

• **Region 3, the 1D TF case:** $N^{-2} \ll g/\bar{\rho} \ll 1$, with $\bar{\rho}$ being of the order $\bar{\rho} \sim (N/L)(NgL)^{-1/(s+1)}$, where s is the degree of homogeneity of the longitudinal confining potential V. This region is described by a Thomas-Fermi type functional

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \int_{-\infty}^{\infty} \left(V_L(z)\rho(z) + \tfrac{1}{2}g\rho(z)^2\right) dz \ . \tag{8.17}$$

It is a limiting case of Region 2 in the sense that $NgL \gg 1$, but a/r is sufficiently small so that $g/\bar{\rho} \ll 1$, i.e., the high density approximation in (8.5) is still valid. The explanation of the factor $(NgL)^{1/(s+1)}$ is as follows: The linear extension $\bar{L}$ of the minimizing density of (8.16) is for large values of NgL determined by $V_L(\bar{L}) \sim g(N/\bar{L})$, which gives $\bar{L} \sim (NgL)^{1/(s+1)}L$. In addition condition (8.15) requires $g\bar{\rho} \ll r^{-2}$, which means that $Na/L(NgL)^{1/(s+1)} \ll 1$. The minimum energy of (8.17) has the scaling property $E^{\mathrm{TF}}(N, L, g) = NL^{-2}(NgL)^{s/(s+1)}E^{\mathrm{TF}}(1, 1, 1)$.

• **Region 4, the LL case:** $g/\bar{\rho} \sim 1$, with $\bar{\rho} \sim (N/L)N^{-2/(s+2)}$, described by an energy functional

$$\mathcal{E}^{\mathrm{LL}}[\rho] = \int_{-\infty}^{\infty} \left(V_L(z)\rho(z) + \rho(z)^3 e(g/\rho(z))\right) dz \ . \tag{8.18}$$

This region corresponds to the case $g/\bar{\rho} \sim 1$, so that neither the high density (8.5) nor the low density approximation (8.6) is valid and the full LL energy (8.4) has to be used. The extension $\bar{L}$ of the system is now determined by $V_L(\bar{L}) \sim (N/\bar{L})^2$ which leads to $\bar{L} \sim LN^{2/(s+2)}$. Condition (8.15) means in this region that $Nr/\bar{L} \sim N^{s/(s+2)}r/L \to 0$. Since $Nr/\bar{L} \sim (\bar{\rho}/g)(a/r)$, this condition is automatically fulfilled if $g/\bar{\rho}$ is bounded away from zero and $a/r \to 0$. The ground state energy of (8.18), $E^{\mathrm{LL}}(N, L, g)$, is equal to $N\gamma^2 E^{\mathrm{LL}}(1, 1, g/\gamma)$, where we introduced the density parameter $\gamma := (N/L)N^{-2/(s+2)}$.

• **Region 5, the GT case:** $g/\bar{\rho} \gg 1$, with $\bar{\rho} \sim (N/L)N^{-2/(s+2)}$, described by a functional with energy density $\sim \rho^3$, corresponding to the Girardeau-Tonks limit of the LL energy density. It corresponds to impenetrable particles, i.e, the limiting case $g/\bar{\rho} \to \infty$ and hence formula (8.6) for the energy density. As in Region 4, the mean density is here $\bar{\rho} \sim \gamma$. The energy functional is

$$\mathcal{E}^{\mathrm{GT}}[\rho] = \int_{-\infty}^{\infty} \left(V_L(z)\rho(z) + (\pi^2/3)\rho(z)^3\right) dz \ , \tag{8.19}$$

with minimum energy $E^{\mathrm{GT}}(N, L) = N\gamma^2 E^{\mathrm{GT}}(1, 1)$.

As already mentioned above, Regions 1–3 can be reached as limiting cases of a 3D Gross-Pitaevskii theory. In this sense, the behavior in these regions contains remnants of the 3D theory, which also shows up in the fact that BEC prevails in Regions 1 and 2 (See [LSeY6] for details.) Heuristically, these traces of 3D can be understood from the fact that in Regions 1–3 the

1D formula for energy per particle, $g\rho \sim aN/(r^2 L)$, gives the same result as the 3D formula, i.e., scattering length times 3D density. This is no longer so in Regions 4 and 5 and different methods are required.

8.2. **Outline of Proof.** We now outline the main steps in the proof of Theorems 8.1 and 8.2, referring to [LSeY6] for full details. To prove (8.11) one has to establish upper and lower bounds, with controlled errors, on the QM many-body energy in terms of the energies obtained by minimizing the energy functionals appropriate for the various regions. The limit theorem for the densities can be derived from the energy estimates in a standard way by variation with respect to the external potential V_L.

The different parameter regions have to be treated by different methods, a watershed lying between Regions 1–3 on the one hand and Regions 4–5 on the other. In Regions 1–3, similar methods as in the proof of the 3D Gross-Pitaevskii limit theorem discussed in Section 6 can be used. This 3D proof needs some modifications, however, because there the external potential was fixed and the estimates are not uniform in the ratio r/L. We will not go into the details here, but mainly focus on Regions 4 and 5, where new methods are needed. It turns out to be necessary to localize the particles by dividing the trap into finite 'boxes' (finite in z-direction), with a controllable particle number in each box. The particles are then distributed optimally among the boxes to minimize the energy, in a similar way as Eq. (2.52) was derived from Eq. (2.47).

A core lemma for Regions 4–5 is an estimate of the 3D ground state energy in a finite box in terms of the 1D energy of the Hamiltonian (8.3). I.e., we will consider the ground state energy of (8.1) with the external potential $V_L(z)$ replaced by a finite box (in z-direction) with length ℓ. Let $E_{\mathrm{D}}^{\mathrm{QM}}(n,\ell,r,a)$ and $E_{\mathrm{N}}^{\mathrm{QM}}(n,\ell,r,a)$ denote its ground state energy with Dirichlet and Neumann boundary conditions, respectively.

Lemma 8.3. *Let $E_{\mathrm{D}}^{\mathrm{1D}}(n,\ell,g)$ and $E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell,g)$ denote the ground state energy of (8.3) on $L^2([0,\ell]^n)$, with Dirichlet and Neumann boundary conditions, respectively, and let g be given by (8.10). Then there is a finite number $C > 0$ such that*

$$E_{\mathrm{N}}^{\mathrm{QM}}(n,\ell,r,a) - \frac{ne^{\perp}}{r^2} \geq E_{\mathrm{N}}^{\mathrm{1D}}(n,\ell,g)\left(1 - Cn\left(\frac{a}{r}\right)^{1/8}\left[1 + \frac{nr}{\ell}\left(\frac{a}{r}\right)^{1/8}\right]\right). \tag{8.20}$$

Moreover,

$$E_{\mathrm{D}}^{\mathrm{QM}}(n,\ell,r,a) - \frac{ne^{\perp}}{r^2} \leq E_{\mathrm{D}}^{\mathrm{1D}}(n,\ell,g)\left(1 + C\left[\left(\frac{na}{r}\right)^2\left(1 + \frac{a\ell}{r^2}\right)\right]^{1/3}\right), \tag{8.21}$$

provided the term in square brackets is less than 1.

This Lemma is the key to the proof of Theorems 8.1 and 8.2. The reader interested in the details is referred to [LSeY6]. Here we only give a sketch of the proof of Lemma 8.3.

Proof of Lemma 8.3. We start with the upper bound (8.21). Let ψ denote the ground state of (8.3) with Dirichlet boundary conditions, normalized by $\langle\psi|\psi\rangle = 1$, and let $\rho_\psi^{(2)}$ denote its two-particle density, normalized by $\int \rho_\psi^{(2)}(z,z')dzdz' = 1$. Let G and F be given by $G(\vec{x}_1,\ldots,\vec{x}_n) = \psi(z_1,\ldots,z_n)\prod_{j=1}^n b_r(\vec{x}_j^\perp)$ and $F(\vec{x}_1,\ldots,\vec{x}_n) = \prod_{i<j} f(|\vec{x}_i - \vec{x}_j|)$. Here f is a monotone increasing function, with $0 \le f \le 1$ and $f(t) = 1$ for $t \ge R$ for some $R \ge R_0$. For $t \le R$ we shall choose $f(t) = f_0(t)/f_0(R)$, where f_0 is the solution to the zero-energy scattering equation for v_a (2.3). Note that $f_0(R) = 1 - a/R$ for $R \ge R_0$, and $f_0'(t) \le t^{-1}\min\{1, a/t\}$. We use as a trial wave function

$$\Psi(\vec{x}_1,\ldots,\vec{x}_n) = G(\vec{x}_1,\ldots,\vec{x}_n)F(\vec{x}_1,\ldots,\vec{x}_n)\ . \tag{8.22}$$

We first have to estimate the norm of Ψ. Using the fact that F is 1 whenever no pair of particles is closer together than a distance R, we obtain

$$\langle\Psi|\Psi\rangle \ge 1 - \frac{n(n-1)}{2}\frac{\pi R^2}{r^2}\|b\|_4^4\ . \tag{8.23}$$

To evaluate the expectation value of the Hamiltonian, we use

$$\langle\Psi| - \Delta_j|\Psi\rangle = -\int F^2 G\Delta_j G + \int G^2|\nabla_j F|^2 \tag{8.24}$$

and the Schrödinger equation $H_{n,g}\psi = E_{\rm D}^{\rm 1D}\psi$. This gives

$$\begin{aligned}\langle\Psi|H|\Psi\rangle &= \left(E_{\rm D}^{\rm 1D} + \frac{n}{r^2}e^\perp\right)\langle\Psi|\Psi\rangle - g\langle\Psi|\sum_{i<j}\delta(z_i - z_j)|\Psi\rangle \\ &\quad + \int G^2\left(\sum_{j=1}^n|\nabla_j F|^2 + \sum_{i<j}v_a(|\vec{x}_i - \vec{x}_j|)|F|^2\right)\ . \end{aligned}\tag{8.25}$$

Now, since $0 \le f \le 1$ and $f' \ge 0$ by assumption, $F^2 \le f(|\vec{x}_i - \vec{x}_j|)^2$, and

$$\sum_{j=1}^n|\nabla_j F|^2 \le 2\sum_{i<j}f'(|\vec{x}_i - \vec{x}_j|)^2 + 4\sum_{k<i<j}f'(|\vec{x}_k - \vec{x}_i|)f'(|\vec{x}_k - \vec{x}_j|)\ . \tag{8.26}$$

Consider the first term on the right side of (8.26), together with the last term in (8.25). These terms are bounded above by

$$n(n-1)\int b_r(\vec{x}^\perp)^2 b_r(\vec{y}^\perp)^2\rho_\psi^{(2)}(z,z')\left(f'(|\vec{x} - \vec{y}|)^2 + \tfrac{1}{2}v_a(|\vec{x} - \vec{y}|)f(|\vec{x} - \vec{y}|)^2\right). \tag{8.27}$$

Let

$$h(z) = \int\left(f'(|\vec{x}|)^2 + \tfrac{1}{2}v_a(|\vec{x}|)f(|\vec{x}|)^2\right)d\vec{x}^\perp\ . \tag{8.28}$$

Using Young's inequality for the integration over the $\perp$-variables, we get

$$(8.27) \leq \frac{n(n-1)}{r^2}\|b\|_4^4 \int_{\mathbb{R}^2} \rho_\psi^{(2)}(z,z')h(z-z')dzdz' \,. \tag{8.29}$$

By similar methods, one can show that the contribution from the last term in (8.26) is bounded by

$$\frac{2}{3}n(n-1)(n-2)\frac{\|b\|_\infty^2}{r^2}\frac{\|b\|_4^4}{r^2}\|k\|_\infty \int_{\mathbb{R}^2} \rho_\psi^{(2)}(z,z')k(z-z')dzdz' \,, \tag{8.30}$$

where

$$k(z) = \int f'(|\vec{x}|)d\vec{x}^\perp \,. \tag{8.31}$$

Note that both h and k are supported in $[-R,R]$.

Now, for any $\phi \in H^1(\mathbb{R})$,

$$\big||\phi(z)|^2 - |\phi(z')|^2\big| \leq 2|z-z'|^{1/2}\left(\int_{\mathbb{R}}|\phi|^2\right)^{1/4}\left(\int_{\mathbb{R}}\left|\frac{d\phi}{dz}\right|^2\right)^{3/4} \,. \tag{8.32}$$

Applying this to $\rho_\psi^{(2)}(z,z')$, considered as a function of z only, we get

$$\begin{aligned}&\int_{\mathbb{R}^2} \rho_\psi^{(2)}(z,z')h(z-z')dzdz' - \int_{\mathbb{R}} h(z)dz \int \rho_\psi^{(2)}(z,z)dz \\ &\leq 2R^{1/2}\int_{\mathbb{R}} h(z)dz \left\langle \psi \left| -\frac{d^2}{dz_1^2}\right| \psi\right\rangle^{3/4} \,,\end{aligned} \tag{8.33}$$

where we used Schwarz's inequality, the normalization of $\rho_\psi^{(2)}$ and the symmetry of ψ. The same argument is used for (8.30) with h replaced by k.

It remains to bound the second term in (8.25). As in the estimate for the norm of Ψ, we use again the fact that F is equal to 1 as long as the particles are not within a distance R. We obtain

$$\langle\Psi|\sum_{i<j}\delta(z_i-z_j)|\Psi\rangle \geq \frac{n(n-1)}{2}\int \rho_\psi^{(2)}(z,z)dz\left(1-\frac{\pi R^2}{r^2}\|b\|_4^4\right) \,. \tag{8.34}$$

We also estimate $g\frac{1}{2}n(n-1)\int\rho_\psi^{(2)}(z,z)dz \leq E_{\mathrm{D}}^{1\mathrm{D}}$ and $\langle\psi| - d^2/dz_1^2|\psi\rangle \leq E_{\mathrm{D}}^{1\mathrm{D}}/n$. We have $\int h(z)dz = 4\pi a(1-a/R)^{-1}$, and the terms containing k can be bounded by $\|k\|_\infty \leq 2\pi a(1+\ln(R/a))/(1-a/r)$ and $\int k(z)dz \leq 2\pi aR(1-a/(2R))/(1-a/r)$. Putting together all the bounds, and choosing

$$R^3 = \frac{ar^2}{n^2(1+g\ell)} \,, \tag{8.35}$$

this proves the desired result.

We are left with the lower bound (8.20). We write a general wave function Ψ as

$$\Psi(\vec{x}_1,\dots,\vec{x}_n) = f(\vec{x}_1,\dots,\vec{x}_n)\prod_{k=1}^n b_r(\vec{x}_k^\perp) \,, \tag{8.36}$$

which can always be done, since b_r is a strictly positive function. Partial integration gives

$$\langle\Psi|H|\Psi\rangle = \frac{ne^{\perp}}{r^2} + \sum_{i=1}^{n} \int \left[|\nabla_i f|^2 + \tfrac{1}{2} \sum_{j,j\neq i} v_a(|\vec{x}_i - \vec{x}_j|)|f|^2 \right] \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k . \tag{8.37}$$

Choose some $R > R_0$, fix i and $\vec{x}_j$, $j \neq i$, and consider the Voronoi cell Ω_j around particle j, i.e., $\Omega_j = \{\vec{x} : |\vec{x} - \vec{x}_j| \leq |\vec{x} - \vec{x}_k| \text{ for all } k \neq j\}$. If $\mathcal{B}_j$ denotes the ball of radius R around $\vec{x}_j$, we can estimate with the aid of Lemma 2.5

$$\begin{aligned} &\int_{\Omega_j \cap \mathcal{B}_j} b_r(\vec{x}_i^{\perp})^2 \left(|\nabla_i f|^2 + \tfrac{1}{2} v_a(|\vec{x}_i - \vec{x}_j|)|f|^2 \right) d\vec{x}_i \\ &\geq \frac{\min_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2}{\max_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2} a \int_{\Omega_j \cap \mathcal{B}_j} b_r(\vec{x}_i^{\perp})^2 U(|\vec{x}_i - \vec{x}_j|)|f|^2 . \end{aligned} \tag{8.38}$$

Here U is given in (2.30). For some $\delta > 0$ let $\mathcal{B}_\delta$ be the subset of $\mathbb{R}^2$ where $b(\vec{x}^{\perp})^2 \geq \delta$, and let $\chi_{\mathcal{B}_\delta}$ denote its characteristic function. Estimating $\max_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2 \leq \min_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2 + 2(R/r^3)\|\nabla b^2\|_\infty$, we obtain

$$\frac{\min_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2}{\max_{\vec{x}\in\mathcal{B}_j} b_r(\vec{x}^{\perp})^2} \geq \chi_{\mathcal{B}_\delta}(\vec{x}_j^{\perp}/r) \left(1 - 2\frac{R}{r} \frac{\|\nabla b^2\|_\infty}{\delta} \right) . \tag{8.39}$$

Denoting $k(i)$ the nearest neighbor to particle i, we conclude that, for $0 \leq \varepsilon \leq 1$,

$$\begin{aligned} &\sum_{i=1}^{n} \int \left[|\nabla_i f|^2 + \tfrac{1}{2} \sum_{j,j\neq i} v_a(|\vec{x}_i - \vec{x}_j|)|f|^2 \right] \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k \\ &\geq \sum_{i=1}^{n} \int \Big[\varepsilon |\nabla_i f|^2 + (1-\varepsilon)|\nabla_i f|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \\ &\qquad + a' U(|\vec{x}_i - \vec{x}_{k(i)}|) \chi_{\mathcal{B}_\delta}(\vec{x}_{k(i)}^{\perp}/r)|f|^2 \Big] \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k , \end{aligned} \tag{8.40}$$

where $a' = a(1-\varepsilon)(1 - 2R\|\nabla b^2\|_\infty / r\delta)$.

Define $F(z_1, \ldots, z_n) \geq 0$ by

$$|F(z_1, \ldots, z_n)|^2 = \int |f(\vec{x}_1, \ldots, \vec{x}_n)|^2 \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k^{\perp} . \tag{8.41}$$

Neglecting the kinetic energy in $\perp$-direction in the second term in (8.40) and using the Schwarz inequality to bound the longitudinal kinetic energy

of f by the one of F, we get the estimate

$$\langle\Psi|H|\Psi\rangle - \frac{ne^{\perp}}{r^2} \geq$$
$$\sum_{i=1}^{n} \int \left[\varepsilon|\partial_i F|^2 + (1-\varepsilon)|\partial_i F|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i)\right] \prod_{k=1}^{n} dz_k$$
$$+ \sum_{i=1}^{n} \int \left[\varepsilon|\nabla_i^{\perp} f|^2 + a'U(|\vec{x}_i - \vec{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\vec{x}_{k(i)}^{\perp}/r)|f|^2\right] \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k, \tag{8.42}$$

where $\partial_j = d/dz_j$, and $\nabla^{\perp}$ denotes the gradient in $\perp$-direction. We now investigate the last term in (8.42). Consider, for fixed $z_1, \ldots, z_n$, the expression

$$\sum_{i=1}^{n} \int \left[\varepsilon|\nabla_i^{\perp} f|^2 + a'U(|\vec{x}_i - \vec{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\vec{x}_{k(i)}^{\perp}/r)|f|^2\right] \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k^{\perp} \,. \tag{8.43}$$

To estimate this term from below, we use Temple's inequality, as in Subsect. 2.2. Let $\widetilde{e}^{\perp}$ denote the gap above zero in the spectrum of $-\Delta^{\perp} + V^{\perp} - e^{\perp}$, i.e., the lowest non-zero eigenvalue. By scaling, $\widetilde{e}^{\perp}/r^2$ is the gap in the spectrum of $-\Delta^{\perp} + V_r^{\perp} - e^{\perp}/r^2$. Note that under the transformation $\phi \mapsto b_r^{-1}\phi$ this latter operator is unitarily equivalent to $\nabla^{\perp *} \cdot \nabla^{\perp}$ as an operator on $L^2(\mathbb{R}^2, b_r(\vec{x}^{\perp})^2 d\vec{x}^{\perp})$, as considered in (8.43). Hence also this operator has $\widetilde{e}^{\perp}/r^2$ as its energy gap. Denoting

$$\langle U^k\rangle = \int \left(\sum_{i=1}^{n} U(|\vec{x}_i - \vec{x}_{k(i)}|)\chi_{\mathcal{B}_\delta}(\vec{x}_{k(i)}^{\perp}/r)\right)^k \prod_{k=1}^{n} b_r(\vec{x}_k^{\perp})^2 d\vec{x}_k^{\perp} \,, \tag{8.44}$$

Temple's inequality implies

$$(8.43) \geq |F|^2 a' \langle U\rangle \left(1 - a' \frac{\langle U^2\rangle}{\langle U\rangle} \frac{1}{\varepsilon \widetilde{e}^{\perp}/r^2 - a'\langle U\rangle}\right) \,. \tag{8.45}$$

Now, using (2.30) and Schwarz's inequality, $\langle U^2\rangle \leq 3n(R^3 - R_0^3)^{-1}\langle U\rangle$, and

$$\langle U\rangle \leq n(n-1)\frac{\|b\|_4^4}{r^2} \frac{3\pi R^2}{R^3 - R_0^3} \,. \tag{8.46}$$

Therefore

$$(8.45) \geq |F|^2 a'' \langle U\rangle \,, \tag{8.47}$$

where we put all the error terms into the modified coupling constant a''. It remains to derive a lower bound on $\langle U\rangle$. Let

$$d(z - z') = \int_{\mathbb{R}^4} b_r(\vec{x}^{\perp})^2 b_r(\vec{y}^{\perp})^2 U(|\vec{x} - \vec{y}|)\chi_{\mathcal{B}_\delta}(\vec{y}^{\perp}/r) d\vec{x}^{\perp} d\vec{y}^{\perp} \,. \tag{8.48}$$

Note that $d(z) = 0$ if $|z| \geq R$. An estimate similar to (2.36) gives

$$\langle U \rangle \geq \sum_{i \neq j} d(z_i - z_j) \left(1 - (n-2) \frac{\pi R^2}{r^2} \|b\|_\infty^2 \right) . \tag{8.49}$$

Note that, for an appropriate choice of R, d is close to a δ-function with the desired coefficient. To make the connection with the δ-function, we can use a bit of the kinetic energy saved in (8.42) to obtain

$$\begin{aligned} &\int \left[\frac{\varepsilon}{n-1} |\partial_i F|^2 + a''' d(z_i - z_j) |F|^2 \right] dz_i \\ &\geq \tfrac{1}{2} g' \max_{|z_i - z_j| \leq R} |F|^2 \chi_{[R, \ell - R]}(z_j) \left(1 - \left(\frac{2(n-1)}{\varepsilon} g' R \right)^{1/2} \right) . \end{aligned} \tag{8.50}$$

Putting all the previous estimates together, we arrive at

$$\begin{aligned} \langle \Psi | H | \Psi \rangle - \frac{n e^\perp}{r^2} \geq & \sum_{i=1}^n \int \left[(1-\varepsilon) |\partial_i F|^2 \chi_{\min_k |z_i - z_k| \geq R}(z_i) \right] \prod_{k=1}^n dz_k \\ & + \sum_{i \neq j} \tfrac{1}{2} g'' \int \max_{|z_i - z_j| \leq R} |F|^2 \chi_{[R, \ell - R]}(z_j) \prod_{k, k \neq i} dz_k \end{aligned} \tag{8.51}$$

for an appropriate coupling constant g'' that contains all the error terms. Now assume that $(n+1)R < \ell$. Given an F with $\int |F|^2 dz_1 \cdots dz_n = 1$, define, for $0 \leq z_1 \leq z_2 \leq \cdots \leq z_n \leq \ell - (n+1)R$,

$$\psi(z_1, \ldots, z_n) = F(z_1 + R, z_2 + 2R, z_3 + 3R, \ldots, z_n + nR) , \tag{8.52}$$

and extend the function to all of $[0, \ell - (n+1)R]^n$ by symmetry. A simple calculation shows that

$$\begin{aligned} (8.51) \geq \langle \psi | H' | \psi \rangle &\geq (1-\varepsilon) E_{\mathrm{N}}^{\mathrm{1D}}(n, \ell - (n+1)R, g'') \langle \psi | \psi \rangle \\ &\geq (1-\varepsilon) E_{\mathrm{N}}^{\mathrm{1D}}(n, \ell, g'') \langle \psi | \psi \rangle , \end{aligned} \tag{8.53}$$

where H' is the Hamiltonian (8.3) with a factor $(1-\varepsilon)$ in front of the kinetic energy term.

It remains to estimate $\langle \psi | \psi \rangle$. Using that F is related to the true ground state Ψ by (8.41), we can estimate it in terms of the total QM energy, namely

$$\begin{aligned} \langle \psi | \psi \rangle \geq & \; 1 - \frac{2R}{g''} \left(E_{\mathrm{N}}^{\mathrm{QM}}(N, \ell, r, a) - \frac{n e^\perp}{r^2} \right) \\ & - 2n \frac{R}{\ell} - 4nR \left(\frac{1}{n} E_{\mathrm{N}}^{\mathrm{QM}}(n, \ell, r, a) - \frac{e^\perp}{r^2} \right)^{1/2} . \end{aligned} \tag{8.54}$$

Collecting all the error terms and choosing

$$R = r \left(\frac{a}{r} \right)^{1/4} , \quad \varepsilon = \left(\frac{a}{r} \right)^{1/8} , \quad \delta = \left(\frac{a}{r} \right)^{1/8} , \tag{8.55}$$

(8.53) and (8.54) lead to the desired lower bound. ∎

As already noted above, Lemma 8.3 is the key to the proof of Theorems 8.1 and 8.2. The estimates are used in each box, and the particles are distributed optimally among the boxes. For the global lower bound, superadditivity of the energy and convexity of the energy density $\rho^3 e(g/\rho)$ are used, generalizing corresponding arguments in Section 2. We refer to [LSeY6] for details.

9. The Charged Bose Gas, the One- and Two-Component Cases

The setting now changes abruptly. Instead of particles interacting with a short-range potential $v(|\vec{x}_i - \vec{x}_j|)$ they interact via the Coulomb potential

$$v(|\vec{x}_i - \vec{x}_j|) = |\vec{x}_i - \vec{x}_j|^{-1}$$

(in 3 dimensions). The unit of electric charge is 1 in our units.

We will here consider both the one- and two-component gases. In the one-component gas (also referred to as the one-component plasma or bosonic jellium) we consider positively charged particles confined to a box with a uniformly charged background. In the two-component gas we have particles of both positive and negative charges moving in all of space.

9.1. **The One-Component Gas.** In the one-component gas there are N positively charged particles in a large box Λ of volume L^3 as before, with $\rho = N/L^3$.

To offset the huge Coulomb repulsion (which would drive the particles to the walls of the box) we add a uniform negative background of precisely the same charge, namely density ρ. Our Hamiltonian is thus

$$H_N^{(1)} = \sum_{i=1}^{N} -\mu\Delta_i - V(\vec{x}_i) + \sum_{1\le i<j\le N} v(|\vec{x}_i - \vec{x}_j|) + C \qquad (9.1)$$

with

$$V(\vec{x}) = \rho \int_\Lambda |\vec{x} - \vec{y}|^{-1} d\vec{y} \qquad \text{and} \qquad C = \frac{1}{2}\rho \int_\Lambda V(\vec{x}) d\vec{x}\,.$$

We shall use Dirichlet boundary conditions. As before the Hamiltonian acts on symmetric wave functions in $L^2(\Lambda^N, d\vec{x}_1 \cdots d\vec{x}_N)$.

Each particle interacts only with others and not with itself. Thus, despite the fact that the Coulomb potential is positive definite, the ground state energy E_0 can be (and is) negative (just take Ψ =const.). This time, *large* ρ is the 'weakly interacting' regime.

We know from the work in [LN] that the thermodynamic limit $e_0(\rho)$ defined as in (2.2) exists. It also follows from this work that we would, in fact, get the same thermodynamic energy if we did not restrict the number of particles N, but considered the grand-canonical case where we minimize the energy over all possible particle numbers, but keeping the background charge ρ fixed.

Another way in which this problem is different from the previous one is that *perturbation theory is correct to leading order.* If one computes $(\Psi, H\Psi)$ with Ψ =const, one gets the right first order answer, namely 0. It is the next order in $1/\rho$ that is interesting, and this is *entirely* due to correlations. In 1961 Foldy [F] calculated this correlation energy according to the prescription of Bogolubov's 1947 theory. That theory was not exact for the dilute Bose gas, as we have seen, even to first order. We are now looking at *second* order, which should be even worse. Nevertheless, there was good physical intuition that this calculation should be asymptotically *exact.* Indeed it is, as proved in [LSo] and [So].

The Bogolubov theory states that the main contribution to the energy comes from pairing of particles into momenta $\vec{k}, -\vec{k}$ and is the bosonic analogue of the BCS theory of superconductivity which came a decade later. I.e., Ψ_0 is a sum of products of terms of the form $\exp\{i\vec{k} \cdot (\vec{x}_i - \vec{x}_j)\}$.

The following theorem is the main result for the one-component gas.

Theorem 9.1 (Foldy's law for the one-component gas).

$$\lim_{\rho\to\infty} \rho^{-1/4} e_0(\rho) = -\frac{2}{5}\frac{\Gamma(3/4)}{\Gamma(5/4)}\left(\frac{2}{\mu\pi}\right)^{1/4}. \tag{9.2}$$

This is the *first example* (in more than 1 dimension) in which Bogolubov's pairing theory has been rigorously validated. It has to be emphasized, however, that Foldy and Bogolubov rely on the existence of Bose-Einstein condensation. We neither make such a hypothesis nor does our result for the energy imply the existence of such condensation. As we said earlier, it is sufficient to prove condensation in small boxes of fixed size.

Incidentally, the one-dimensional example for which Bogolubov's theory is asymptotically exact to the first two orders (high density) is the repulsive delta-function Bose gas [LL], for which there is no Bose-Einstein condensation.

To appreciate the $-\rho^{1/4}$ nature of (9.2), it is useful to compare it with what one would get if the bosons had infinite mass, i.e., the first term in (9.1) is dropped. Then the energy would be proportional to $-\rho^{1/3}$ as shown in [LN]. Thus, the effect of quantum mechanics is to lower $\frac{1}{3}$ to $\frac{1}{4}$.

A problem somewhat related to bosonic jellium is *fermionic* jellium. Graf and Solovej [GS] have proved that the first two terms are what one would expect, namely

$$e_0(\rho) = C_{\mathrm{TF}}\rho^{5/3} - C_{\mathrm{D}}\rho^{4/3} + o(\rho^{4/3}), \tag{9.3}$$

where C_{TF} is the usual Thomas-Fermi constant and C_{D} is the usual Dirac exchange constant.

It is supposedly true, for both bosonic and fermionic particles, that there is a critical mass above which the ground state should show crystalline ordering (Wigner crystal), but this has never been proved and it remains an intriguing open problem, even for the infinite mass case. A simple scaling

shows that large mass is the same as small ρ, and is thus outside the region where a Bogolubov approximation can be expected to hold.

As for the dilute Bose gas, there are several relevant length scales in the problem of the charged Bose gas. For the dilute gas there were three scales. This time there are just two. Because of the long range nature of the Coulomb problem there is no scale corresponding to the scattering length a. One relevant length scale is again the interparticle distance $\rho^{-1/3}$. The other is the correlation length scale $\ell_{\rm cor} \sim \rho^{-1/4}$ (ignoring the dependence on μ). The order of the correlation length scale can be understood heuristically as follows. Localizing on a scale $\ell_{\rm cor}$ requires kinetic energy of the order of $\ell_{\rm cor}^{-2}$. The Coulomb potential from the particles and background on the scale $\ell_{\rm cor}$ is $(\rho\ell_{\rm cor}^3)/\ell_{\rm cor}$. Thus the kinetic energy and the Coulomb energy balance when $\ell_{\rm cor} \sim \rho^{-1/4}$. This heuristics is however much too simplified and hides the true complexity of the situation.

Note that in the high density limit $\ell_{\rm cor}$ is long compared to the interparticle distance. This is analogous to the dilute gas where the scale ℓ_c is also long compared to the interparticle distance [see (2.12)]. There is however no real analogy between the scale $\ell_{\rm cor}$ for the charged gas and the scale ℓ_c for the dilute gas. In particular, whereas $e_0(\rho)$ for the dilute gas is, up to a constant, of the same order as the kinetic energy $\sim \mu\ell_c^{-2}$ we have for the charged gas that $e_0(\rho) \not\sim \ell_{\rm cor}^{-2} = \rho^{1/2}$. The reason for this difference is that on average only a small fraction of the particles in the charged gas actually correlate.

9.2. **The Two-Component Gas.** Now we consider N particles with charges ± 1. The Hamiltonian is thus

$$H_N^{(2)} = \sum_{i=1}^{N} -\mu\Delta_i + \sum_{1\le i<j\le N} \frac{e_i e_j}{|\vec{x}_i - \vec{x}_j|}.$$

This time we are interested in $E_0^{(2)}(N)$ the ground state energy of $H_N^{(2)}$ minimized over all possible combination of charges $e_i = \pm 1$, i.e., we do not necessarily assume that the minimum occurs for the neutral case. Restricting to the neutral case would however not change the result we give below.

An equivalent formulation is to say that $E_0^{(2)}(N)$ is the ground state energy of the Hamiltonian acting on all wave functions of space and charge, i.e., functions in $L^2\left((\mathbb{R}^3 \times \{-1,1\})^N\right)$. As mentioned in the introduction, and explained in the beginning of the proof of Thm. 2.2, for the calculation of the ground state energy we may as usual restrict to symmetric functions in this Hilbert space.

For the two-component gas there is no thermodynamic limit. In fact, Dyson [D2] proved that $E_0^{(2)}(N)$ was at least as negative as $-(\text{const})N^{7/5}$ as $N \to \infty$. Thus, thermodynamic stability (i.e., a linear lower bound) fails for this gas. Years later, a lower bound of this $-N^{7/5}$ form was finally established in [CLY], thereby proving that this law is correct.

The connection of this $-N^{7/5}$ law with the jellium $-\rho^{1/4}$ law (for which a corresponding lower bound was also given in [CLY]) was pointed out by Dyson [D2] in the following way. Assuming the correctness of the $-\rho^{1/4}$ law, one can treat the 2-component gas by treating each component as a background for the other. What should the density be? If the gas has a radius L and if it has N bosons then $\rho = NL^{-3}$. However, the extra kinetic energy needed to compress the gas to this radius is NL^{-2}. The total energy is then $NL^{-2} - N\rho^{1/4}$, and minimizing this with respect to L gives $L \sim N^{-1/5}$ and leads to the $-N^{7/5}$ law. The correlation length scale is now $\ell_{\text{cor}} \sim \rho^{-1/4} \sim N^{-2/5}$.

In [D2] Dyson conjectured an exact asymptotic expression for $E_0^{(2)}(N)$ for large N. That this asymptotics, as formulated in the next theorem, is indeed correct is proved in [LSo2] and [So].

Theorem 9.2 (Dyson's law for the two-component gas).

$$\lim_{N\to\infty} \frac{E_0^{(2)}(N)}{N^{7/5}} = \inf\left\{ \mu \int_{\mathbb{R}^3} |\nabla\Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2} \;\middle|\; 0 \le \Phi,\ \int_{\mathbb{R}^3} \Phi^2 = 1 \right\}, \quad (9.4)$$

where I_0 is the constant from Foldy's law:

$$I_0 = \frac{2}{5}\frac{\Gamma(3/4)}{\Gamma(5/4)} \left(\frac{2}{\mu\pi}\right)^{1/4}.$$

This asymptotics can be understood as a mean field theory for the gas density, very much like the Gross-Pitaevskii functional for dilute trapped gases, where the local energy described by Foldy's law should be balanced by the kinetic energy of the gas density. Thus if we let the gas density be given by ϕ^2 then the "mean field" energy should be

$$\mu \int_{\mathbb{R}^3} |\nabla\phi|^2 - I_0 \int_{\mathbb{R}^3} \phi^{5/2}. \quad (9.5)$$

Here $\int \phi^2 = N$. If we now define $\Phi(\vec{x}) = N^{-8/5}\phi(N^{-1/5}\vec{x})$ we see that $\int \Phi^2 = 1$ and that the above energy is

$$N^{7/5}\left(\mu \int_{\mathbb{R}^3} |\nabla\Phi|^2 - I_0 \int_{\mathbb{R}^3} \Phi^{5/2}\right).$$

It may be somewhat surprising that it is exactly the same constant I_0 that appears in both the one- and two-component cases. The reason that there are no extra factors to account for the difference between one and two components is, as we shall see below, a simple consequence of Bogolubov's method. The origin of this equivalence, while clear mathematically, does not appear to have a simple physical interpretation.

9.3. **The Bogolubov Approximation.** In this section we shall briefly explain the Bogolubov approximation and how it is applied in the case of the charged Bose gas. The Bogolubov method relies on the exact diagonalization of a Hamiltonian, which is quadratic in creation and annihilation operators. For the charged Bose gas one only needs a very simple case of the general

diagonalization procedure. On the other hand, the operators that appear are not exact creation and annihilation operators. A slightly more general formulation is needed.

Theorem 9.3 (Simple case of Bogolubov's method).
Assume that $b_{\pm,\pm}$ are four (possibly unbounded) commuting operators satisfying the operator inequality

$$\left[b_{\tau,e}, b^*_{\tau,e}\right] \leq 1 \quad \text{for all } e, \tau = \pm.$$

Then for all real numbers $\mathcal{A}, \mathcal{B}_+, \mathcal{B}_- \geq 0$ we have

$$\begin{aligned}
&\mathcal{A} \sum_{\tau,e=\pm 1} b^*_{\tau,e} b_{\tau,e} \\
&\quad + \sum_{e,e'=\pm 1} \sqrt{\mathcal{B}_e \mathcal{B}_{e'}}\, ee' (b^*_{+,e} b_{+,e'} + b^*_{-,e} b_{-,e'} + b^*_{+,e} b^*_{-,e'} + b_{+,e} b_{-,e'}) \\
&\geq -(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-) + \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2}.
\end{aligned}$$

If $b_{\pm,\pm}$ are four annihilation operators then the lower bound is sharp.

Proof. Let us introduce

$$d^*_\pm = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_+^{1/2} b^*_{\pm,+} - \mathcal{B}_-^{1/2} b^*_{\pm,-}),$$

and

$$c^*_\pm = (\mathcal{B}_+ + \mathcal{B}_-)^{-1/2} (\mathcal{B}_-^{1/2} b^*_{\pm,+} + \mathcal{B}_+^{1/2} b^*_{\pm,-}).$$

Then these operators satisfy

$$[d_+, d^*_+] \leq 1, \quad [d_-, d^*_-] \leq 1.$$

The operator that we want to estimate from below may be rewritten as

$$\begin{aligned}
&\mathcal{A}(d^*_+ d_+ + d^*_- d_- + c^*_+ c_+ + c^*_- c_-) \\
&+(\mathcal{B}_+ + \mathcal{B}_-)\left(d^*_+ d_+ + d^*_- d_- + d^*_+ d^*_- + d_+ d_-\right).
\end{aligned}$$

We may now complete the squares to write this as

$$\begin{aligned}
&\mathcal{A}(c^*_+ c_+ + c^*_- c_-) + D(d^*_+ + \lambda d_-)(d^*_+ + \lambda d_-)^* \\
&+D(d^*_- + \lambda d_+)(d^*_- + \lambda d_+)^* - D\lambda^2([d_+, d^*_+] + [d_-, d^*_-])
\end{aligned}$$

if

$$D(1 + \lambda^2) = \mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-, \quad 2D\lambda = \mathcal{B}_+ + \mathcal{B}_-.$$

We choose the solution $\lambda = 1 + \frac{\mathcal{A}}{\mathcal{B}_+ + \mathcal{B}_-} - \sqrt{\left(1 + \frac{\mathcal{A}}{(\mathcal{B}_+ + \mathcal{B}_-)}\right)^2 - 1}$. Hence

$$D\lambda^2 = \tfrac{1}{2}\left(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_- - \sqrt{(\mathcal{A} + \mathcal{B}_+ + \mathcal{B}_-)^2 - (\mathcal{B}_+ + \mathcal{B}_-)^2}\right).$$

■

In the theorem above one could of course also have included linear terms in $b_{\tau,e}$ in the Hamiltonian. In the technical proofs in [LSo, LSo2] the Bogolubov diagonalization with linear terms is indeed being used to control certain error terms. Here we shall not discuss the technical details of the proofs. We have therefore stated the theorem in the simplest form in which we shall need it to derive the leading contribution.

In our applications to the charged Bose gas the operators $b_{\pm,e}$ will correspond to the annihilation of particles with charge $e = \pm$ and momenta $\pm k$ for some $k \in \mathbb{R}^3$. Thus, only equal and opposite momenta couple. In a translation invariant case this would be a simple consequence of momentum conservation. The one-component gas is not translation invariant, in our formulation. The two-component gas is translation invariant, but it is natural to break translation invariance by going into the center of mass frame. In both cases it is only in some approximate sense that equal and opposite momenta couple.

In the case of the one-component gas we only need particles of one sign. In this case we use the above theorem with $b_{\pm,-} = 0$ and $\mathcal{B}_- = 0$.

We note that the lower bounds in Theorem 9.3 for the one- and two-component gases are the same except for the replacement of $\mathcal{B}_+$ in the one-component case by $\mathcal{B}_+ + \mathcal{B}_-$ in the two-component case. In the application to the two-component gas $\mathcal{B}_+$ and $\mathcal{B}_-$ will be proportional to the particle densities for respectively the positive or negatively charged particles. For the one-component gas $\mathcal{B}_+$ is proportional to the background density.

The Bogolubov diagonalization method cannot be immediately applied to the operators $H_N^{(1)}$ or $H_N^{(2)}$ since these operators are *not* quadratic in creation and annihilation operators. In fact, they are quartic. They have the general form

$$\sum_{\alpha,\beta} t_{\alpha\beta} a_\alpha^* a_\beta + \tfrac{1}{2} \sum_{\alpha,\beta,\mu,\nu} w_{\alpha\beta\mu\nu} a_\alpha^* a_\beta^* a_\nu a_\mu, \tag{9.6}$$

with

$$t_{\alpha\beta} = \langle \alpha | T | \beta \rangle, \qquad w_{\alpha\beta\mu\nu} = \langle \alpha\beta | W | \mu\nu \rangle,$$

where T is the one-body part of the Hamiltonian and W is the two-body-part of the Hamiltonian.

The main step in Bogolubov's approximation is now to assume Bose-Einstein condensation, i.e., that almost all particles are in the same one-particle state. In case of the two-component gas this means that almost half the particles are positively charged and in the same one-particle state as almost all the other half of negatively charged particles. We denote this condensate state by the index $\alpha = 0$ in the sums above. Based on the assumption of condensation Bogolubov now argues that one may ignore all terms in the quartic Hamiltonian above which contain 3 or 4 non-zero indices and at the same time replace all creation and annihilation operators of the condensate by their expectation values. The result is a quadratic Hamiltonian (including linear terms) in the creation and annihilation with non-zero

index. This Hamiltonian is of course not particle number preserving, reflecting the simple fact that particles may be created out of the condensate or annihilated into the condensate.

In Section 9.5 below it is explained how to construct trial wave functions for the one- and two-component charged gases whose expectations agree essentially with the prescription in the Bogolubov approximation. The details are to appear in [So]. This will imply upper bounds on the energies corresponding to the asymptotic forms given in Theorems 9.1 and 9.2.

In [LSo, LSo2] it is proved how to make the steps in the Bogolubov approximation rigorous as lower bounds. The main difficulty is to control the degree of condensation. As already explained it is not necessary to prove condensation in the strong sense described above. We shall only prove condensation in small boxes. Put differently, we shall not conclude that most particles are in the same one-particle state, but rather prove that most particles occupy one-particle states that look the same on short scales, i.e., that vary slowly. Here the short scale is the correlation length scale $\ell_{\rm cor}$.

9.4. **The Rigorous Lower Bounds.** As already mentioned we must localize into small boxes of some fixed size ℓ. This time we must require $\ell_{\rm cor} \ll \ell$. For the one-component gas this choice is made only in order to control the degree of condensation. For the two-component gas it is required both to control the order of condensation, and also to make a local constant density approximation. The reason we can control the degree of condensation in a small box is that the localized kinetic energy has a gap above the lowest energy state. In fact, the gap is of order ℓ^{-2}. Thus if we require that ℓ is such that $N\ell^{-2}$ is much greater than the energy we may conclude that most particles are in the lowest eigenvalue state for the localized kinetic energy. We shall always choose the localized kinetic energy in such a way that the lowest eigenstate, and hence the condensate, is simply a constant function.

9.4.1. *Localizing the interaction.* In contrast to the dilute gas the long range Coulomb potential prevents us from simply ignoring the interaction between the small boxes. To overcome this problem we use a sliding technique first introduced in [CLY].

Theorem 9.4 (Controlling interactions by sliding). *Let χ be a smooth approximation to the characteristic function of the unit cube centered at the origin. For $\ell > 0$ and $\vec{z} \in \mathbb{R}^3$ let $\chi_{\vec{z}}(\vec{x}) = \chi((\vec{x}-\vec{z})/\ell)$. There exists an $\omega > 0$ depending on χ (in such a way that it tends to infinity as χ approximates the characteristic function) such that*

$$\sum_{1\le i<j\le N} \frac{e_i e_j}{|\vec{x}_i - \vec{x}_j|} \ge \left(\int \chi^2\right)^{-1} \int_{\mathbb{R}^3} \sum_{1\le i<j\le N} e_i e_j w_{\ell\vec{z}}(\vec{x}_i, \vec{x}_j) d\vec{z} - \frac{N\omega}{2\ell},$$

for all $\vec{x}_1, \ldots \in \mathbb{R}^3$ and $e_1, \ldots = \pm 1$, where

$$w_{\vec{z}}(\vec{x}, \vec{y}) = \chi_{\vec{z}}(\vec{x}) Y_{\omega/\ell}(\vec{x} - \vec{y}) \chi_{\vec{z}}(\vec{y})$$

with $Y_\mu(\vec{x}) = |\vec{x}|^{-1}\exp(-\mu|\vec{x}|)$ *being the Yukawa potential.*

The significance of this result is that the two-body potential $w_{\vec{z}}$ is localized to the cube of size ℓ centered at $\ell\vec{z}$. The lower bound above is thus an integral over localized interactions sliding around with the integration parameter.

We have stated the sliding estimate in the form relevant to the two-component problem. There is an equivalent version for the one-component gas, where the sum of the particle-particle, particle-background, and background-background interactions may be bounded below by corresponding localized interactions.

Since $\ell \gg \ell_{\text{cor}}$ the error in the sliding estimate is much smaller than $\omega N/\ell_{\text{cor}}$, which for both the one and two-component gases is of order ω times the order of the energy. Thus, since ℓ is much bigger than ℓ_{cor}, we have room to let ω be very large, i.e., χ is close to the characteristic function.

9.4.2. *Localizing the kinetic energy.* Having described the technique to control the interaction between localized regions we turn next to the *localization of the kinetic energy.*

For the two-component gas this is done in two steps. As already mentioned it is natural to break the translation invariance of the two-component gas. We do this by localizing the system into a box of size $L' \gg N^{-1/5}$ (which as we saw is the expected size of the gas) as follows. By a partition of unity we can divide space into boxes of this size paying a localization error due to the kinetic energy of order $NL'^{-2} \ll N^{7/5}$. We control the interaction between these boxes using the sliding technique.

We may now argue, as follows, that the energy is smallest if all the particles are in just one box. For simplicity we give this argument for the case of two boxes. Suppose the two boxes have respective wave functions ψ and $\widetilde{\psi}$. The total energy of these two non-interacting boxes is $E + \widetilde{E}$. Now put all the particles in one box with the trial function $\Psi = \psi\widetilde{\psi}$. The fact that this function is not bosonic (i.e., it is not symmetric with respect to all the variables) is irrelevant because the true bosonic ground state energy is never greater than that of any trial state (Perron-Frobenius Theorem). The energy of Ψ is

$$E + \widetilde{E} + \iint \rho_\psi(\vec{x})|\vec{x} - \vec{y}|^{-1}\rho_{\widetilde{\psi}}(\vec{y})d\vec{x}d\vec{y},$$

where ρ_ψ and $\rho_{\widetilde{\psi}}$ are the respective *charge* densities of the states ψ and $\widetilde{\psi}$. We claim that the last Coulomb term can be made non-positive. How? If it is positive then we simply change the state $\widetilde{\psi}$ by interchanging positive and negative charges (only in $\widetilde{\psi}$ and not in ψ). The reader is reminded that we have not constrained the number of positive and negative particles but only their sum. This change in $\widetilde{\psi}$ reverses the relative charge of the states ψ and $\widetilde{\psi}$ so, by symmetry the energies E and $\widetilde{E}$ do not change, whereas the Coulomb interaction changes sign.

The localization into smaller cubes of size ℓ can however not be done by a crude partition of unity localization. Indeed, this would cost a localization error of order $N\ell^{-2}$, which as explained is required to be of much greater order than the energy.

For the one-component charged gas we may instead use a Neumann localization of the kinetic energy, as for the dilute Bose gas. If we denote by $\Delta_\ell^{(\vec{z})}$ the Neumann Laplacian for the cube of size ℓ centered at $\vec{z}$ we may, in the spirit of the sliding estimate, write the Neumann localization Laplacian in all of $\mathbb{R}^3$ as

$$-\Delta = \int -\Delta_\ell^{(\ell\vec{z})} d\vec{z}.$$

In order to write the localized kinetic energy in the same form as the localized interaction we must introduce the smooth localization χ as in Theorem 9.4. This can be achieved by ignoring the low momentum part of the kinetic energy.

More precisely, there exist $\varepsilon(\chi)$ and $s(\chi)$ such that $\varepsilon(\chi) \to 0$ and $s(\chi) \to 0$ as χ approaches the characteristic function of the unit cube and such that (see Lemma 6.1 in [LSo])

$$-\Delta_\ell^{(\vec{z})} \geq (1-\varepsilon(\chi))\mathcal{P}_{\vec{z}}\chi_{\vec{z}}(\vec{x})F_{\ell s(\chi)}(-\Delta)\chi_{\vec{z}}(\vec{x})\mathcal{P}_{\vec{z}} \tag{9.7}$$

where $\mathcal{P}_{\vec{z}}$ denotes the projection orthogonal to constants in the cube of size ℓ centered at z and

$$F_s(u) = \frac{u^2}{u+s^{-2}}.$$

For $u \ll s^{-2}$ we have that $F_s(u) \ll u$. Hence the effect of F in the operator estimate above is to ignore the low momentum part of the Laplacian.

For the two-component gas one cannot use the Neumann localization as for the one-component gas. Using a Neumann localization ignores the kinetic energy corresponding to long range variations in the wave function and one would not get the kinetic energy term $\int \mu|\nabla\Phi|^2$ in (9.4). This is the essential difference between the one- and two-component cases. This problem is solved in [LSo2] where a new kinetic energy localization technique is developed. The idea is again to separate the high and low momentum part of the kinetic energy. The high momentum part is then localized as before, whereas the low momentum part is used to connect the localized regions by a term corresponding to a discrete Laplacian. (For details and the proof the reader is referred to [LSo2].)

Theorem 9.5 (A many body kinetic energy localization). *Let $\chi_{\vec{z}}$, $\mathcal{P}_{\vec{z}}$ and F_s be as above. There exist $\varepsilon(\chi)$ and $s(\chi)$ such that $\varepsilon(\chi) \to 0$ and $s(\chi) \to 0$ as χ approaches the characteristic function of the unit cube and such that for all normalized symmetric wave functions Ψ in $L^2((\mathbb{R}^3 \times$*

$\{-1,1\})^N)$ *and all* $\Omega \subset \mathbb{R}^3$ *we have*

$$(1+\varepsilon(\chi))\left(\Psi, \sum_{i=1}^{N} -\Delta_i \Psi\right) \geq \int_\Omega \Big[(\Psi, \mathcal{P}_{\ell\vec{z}}\chi_{\ell\vec{z}}(\vec{x})F_{\ell s(\chi)}(-\Delta)\chi_{\ell\vec{z}(\vec{x})}\mathcal{P}_{\ell\vec{z}}\Psi) + \tfrac{1}{2}\ell^{-2}\sum_{\substack{\vec{y}\in\mathbb{Z}^3 \\ |\vec{y}|=1}} (S_\Psi(\ell(\vec{z}+\vec{y})) - S_\Psi(\ell\vec{z}))^2\Big] d\vec{z} - \text{const.}\,\ell^{-2}\text{Vol}(\Omega),$$

where

$$S_\Psi(\vec{z}) = \sqrt{(\Psi, (a_{0+}^*(\vec{z})a_{0+}(\vec{z}) + a_{0-}^*(\vec{z})a_{0-}(\vec{z}))\Psi) + 1} - 1$$

with $a_{0\pm}(z)$ *being the annihilation of a particle of charge* $\pm$ *in the state given by the normalized characteristic function of the cube of size* ℓ *centered at* $\vec{z}$.

The first term in the kinetic energy localization in this theorem is the same as in (9.7). The second term gives rise to a discrete Laplacian for the function $S_\Psi(\ell\vec{z})$, which is essentially the number of condensate particles in the cube of size ℓ centered at $\ell\vec{z}$. Since we will eventually conclude that most particles are in the condensate this term will after approximating the discrete Laplacian by the continuum Laplacian lead to the term $\int \mu|\nabla\phi|^2$ in (9.5). We shall not discuss this any further here.

When we apply this theorem to the two-component gas the set $\ell\Omega$ will be the box of size L' discussed above. Hence the error term $\ell^{-2}\text{Vol}(\Omega)$ will be of order $L'^3/\ell^{-5} \ll (N^{2/5}\ell)^{-5}(N^{1/5}L')^3 N^{7/5}$. Thus since $\ell \gg N^{-2/5}$ we may still choose $L' \gg N^{-1/5}$, as required, and have this error term be lower order than $N^{7/5}$.

9.4.3. *Controlling the degree of condensation.* After now having localized the problem into smaller cubes we are ready to control the degree of condensation. We recall that the condensate state is the constant function in each cube. Let us denote by $\widehat{n}_{\vec{z}}$ the number of excited (i.e., non-condensed particles) in the box of size ℓ centered at $\vec{z}$. Thus for the two-component gas $\widehat{n}_{\vec{z}} + a_{0+}^*(\vec{z})a_{0+}(\vec{z}) + a_{0-}^*(\vec{z})a_{0-}(\vec{z})$ is the total number of particles in the box and a similar expression gives the particle number for the one-component gas.

As discussed above we can use the fact that the kinetic energy localized to a small box has a gap above its lowest eigenvalue to control the number of excited particles. Actually, this will show that the expectation $(\Psi, \widehat{n}_{\vec{z}}\Psi)$ is much smaller than the total number of particles in the box for any state Ψ with negative energy expectation.

One needs, however, also a good bound on $(\Psi, \widehat{n}_{\vec{z}}^2\Psi)$ to control the Coulomb interaction of the non-condensed particles. This is more difficult. In [LSo] this is not achieved directly through a bound on $(\Psi, \widehat{n}_{\vec{z}}\Psi)$ in the ground state. Rather it is proved that one may change the ground state without changing its energy very much, so that it only contains values of $\widehat{n}_{\vec{z}}$

localized close to $(\Psi, \widehat{n}_{\vec{z}}\Psi)$. The following theorem gives this very general localization technique. Its proof can be found in [LSo].

Theorem 9.6 (Localizing large matrices). *Suppose that $\mathcal{A}$ is an $N+1 \times N+1$ Hermitean matrix and let $\mathcal{A}^k$, with $k = 0, 1, ..., N$, denote the matrix consisting of the k^{th} supra- and infra-diagonal of $\mathcal{A}$. Let $\psi \in \mathbf{C}^{N+1}$ be a normalized vector and set $d_k = (\psi, \mathcal{A}^k\psi)$ and $\lambda = (\psi, \mathcal{A}\psi) = \sum_{k=0}^{N} d_k$. ($\psi$ need not be an eigenvector of $\mathcal{A}$.)*

Choose some positive integer $M \leq N+1$. Then, with M fixed, there is some $n \in [0, N+1-M]$ and some normalized vector $\phi \in \mathbf{C}^{N+1}$ with the property that $\phi_j = 0$ unless $n+1 \leq j \leq n+M$ (i.e., ϕ has length M) and such that

$$(\phi, \mathcal{A}\phi) \leq \lambda + \frac{C}{M^2} \sum_{k=1}^{M-1} k^2 |d_k| + C \sum_{k=M}^{N} |d_k| \,, \tag{9.8}$$

where $C > 0$ is a universal constant. (Note that the first sum starts with $k = 1$.)

To use this theorem we start with a ground state (or approximate ground state) Ψ to the many body problem. We then consider the projections of Ψ onto the eigenspaces of $\widehat{n}_{\vec{z}}$. Since the possible eigenvalues run from 0 to N these projections span an at most $N+1$ dimensional space.

We use the above theorem with $\mathcal{A}$ being the many body Hamiltonian restricted to this $N+1$ dimensional subspace. Since the Hamiltonian can change the number of excited particles by at most two we see that d_k vanishes for $k \geq 3$. We shall not here discuss the estimates on d_1 and d_2 (see [LSo, LSo2]). The conclusion is that we may, without changing the energy expectation of Ψ too much, assume that the values of $\widehat{n}_{\vec{z}}$ run in an interval of length much smaller than the total number of particles. We would like to conclude that this interval is close to zero. This follows from the fact that any wave function with energy expectation close to the minimum must have an expected number of excited particles much smaller than the total number of particles.

9.4.4. *The quadratic Hamiltonian.* Using our control on the degree of condensation it is now possible to estimate all unwanted terms in the Hamiltonian, i.e., terms that contain 3 or more creation or annihilation operators corresponding to excited (non-condensate) states. The proof which is a rather complicated bootstrapping argument is more or less the same for the one- and two-component gases. The result, in fact, shows that we can ignore other terms too. In fact if we go back to the general form (9.6) of the Hamiltonian it turns out that we can control all quartic terms except the ones with the coefficients:

$$w_{\alpha\beta 00},\ w_{00\alpha\beta},\ w_{\alpha 00\beta},\ \text{and}\ w_{0\alpha\beta 0}.$$

To be more precise, let u_α, $\alpha = 1, \ldots$ be an orthonormal basis of real functions for the subspace of functions on the cube of size ℓ centered at $\vec{z}$ orthogonal to constants, i.e, with vanishing average in the cube. We shall now omit the subscript $\vec{z}$ and let $a_{0\pm}$ be the annihilation of a particle of charge ± 1 in the normalized constant function in the cube (i.e., in the condensate). Let $a_{\alpha\pm}$ with $\alpha \neq 0$ be the annihilation operator for a particle of charge ± 1 in the state u_α. We can then show that the main contribution to the localized energy of the two-component gas comes from the Hamiltonian

$$H_{\text{local}} = \sum_{\substack{\alpha,\beta=1 \\ e=\pm 1}}^{\infty} t_{\alpha\beta} a^*_{\alpha e} a_{\beta e}$$
$$+ \tfrac{1}{2} \sum_{\substack{\alpha,\beta=1 \\ e,e'=\pm 1}} e e' w_{\alpha\beta} (2a^*_{0e} a^*_{\alpha e'} a_{0e'} a_{\beta e} + a^*_{0e} a^*_{0e'} a_{\alpha e'} a_{\beta e} + a^*_{\alpha e} a^*_{\beta e'} a_{0e'} a_{0e}),$$

where

$$t_{\alpha\beta} = \mu(u_\alpha, \mathcal{P}_{\vec{z}} \chi_{\vec{z}}(\vec{x}) F_{\ell s(\chi)}(-\Delta) \chi_{\vec{z}}(\vec{x}) \mathcal{P}_{\vec{z}} u_\beta)$$

and

$$w_{\alpha\beta} = \ell^{-3} \iint u_\alpha(\vec{x}) \chi_{\vec{z}}(\vec{x}) Y_{\omega/\ell}(\vec{x} - \vec{y}) \chi_{\vec{z}}(\vec{y}) u_\beta(\vec{x}) d\vec{x} d\vec{y}.$$

In H_{local} we have ignored all error terms and hence also $\varepsilon(\chi) \approx 0$ and $\int \chi^2 \approx 1$.

In the case of the one-component gas we get exactly the same local Hamiltonian, except that we have only one type of particles, i.e, we may set $a_{\alpha-} = 0$ above.

Let $\nu_\pm = \sum_{\alpha=0}^{\infty} a^*_{\alpha\pm} a_{\alpha\pm}$ be the total number of particles in the box with charge ± 1. For $\vec{k} \in \mathbb{R}^3$ we let $\chi_{\vec{k},\vec{z}}(\vec{x}) = \chi_{\vec{z}}(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$. We then introduce the operators

$$b_{\vec{k}\pm} = (\ell^3 \nu_\pm)^{-1/2} a_\pm(\mathcal{P}_{\vec{z}} \chi_{\vec{k},\vec{z}}) a^*_{0\pm},$$

where $a_\pm(\mathcal{P}_{\vec{z}} \chi_{\vec{k},\vec{z}}) = \sum_{\alpha=1}^{\infty} (\chi_{\vec{k},\vec{z}}, u_\alpha) a_{\alpha\pm}$ annihilates a particle in the state $\chi_{\vec{k},\vec{z}}$ with charge ± 1. It is then clear that the operators $b_{\vec{k}\pm}$ all commute and a straightforward calculation shows that

$$[b_{\vec{k}\pm}, b^*_{\vec{k}\pm}] \leq (\ell^3 \nu_\pm)^{-1} \|\mathcal{P}_{\vec{z}} \chi_{\vec{z}}\|^2 a^*_{0\pm} a_{0\pm} \leq 1.$$

If we observe that

$$\sum_{\substack{\alpha,\beta=1 \\ e=\pm 1}}^{\infty} t_{\alpha\beta} a^*_{\alpha e} a_{\beta e} = (2\pi)^{-3} \int \mu F_{\ell s(\chi)}(\vec{k}^2) \sum_{e=\pm} a_e(\mathcal{P}_{\vec{z}} \chi_{\vec{k},\vec{z}})^* a_e(\mathcal{P}_{\vec{z}} \chi_{\vec{k},\vec{z}}) d\vec{k}$$
$$\geq (2\pi)^{-3} \ell^3 \int \mu F_{\ell s(\chi)}(\vec{k}^2) \sum_{e=\pm} b^*_{\vec{k}e} b_{\vec{k}e},$$

we see that

$$H_{\text{local}} \geq \tfrac{1}{2}(2\pi)^{-3} \int \mu\ell^3 F_{\ell s(\chi)}(\vec{k}^2) \sum_{e=\pm} (b^*_{\vec{k}e} b_{\vec{k}e} + b^*_{-\vec{k}e} b_{-\vec{k}e})$$
$$+ \sum_{ee'=\pm} \widehat{Y}_{\omega/\ell}(\vec{k}) \sqrt{\nu_e \nu_{e'}}\, ee' (b^*_{\vec{k}e} b_{\vec{k},e'} + b^*_{-\vec{k}e} b_{-\vec{k},e'} + b^*_{\vec{k}e} b^*_{-\vec{k},e'} + b_{-\vec{k}e} b_{\vec{k},e'}) d\vec{k}$$
$$- \sum_{\alpha\beta=1} w_{\alpha\beta} (a^*_{\alpha+} a_{\beta+} + a^*_{\alpha-} a_{\beta-})$$

The last term comes from commuting $a^*_{0\pm} a_{0\pm}$ to $a_{0\pm} a^*_{0\pm}$. It is easy to see that this last term is a bounded operator with norm bounded by

$$\text{const.}\,(\nu_+ + \nu_-)\ell^{-3} \|\widehat{Y}_{\omega/\ell}\|_\infty \leq \text{const.}\,\omega^{-2}(\nu_+ + \nu_-)\ell^{-1}.$$

When summing over all boxes we see that the last term above gives a contribution bounded by $\text{const.}\,\omega^{-2} N \ell^{-1} = \omega^{-2}(N^{2/5}\ell)^{-1} N^{7/5}$ which is lower order than the energy.

The integrand in the lower bound on H_{local} is precisely an operator of the form treated in the Bogolubov method Theorem 9.3. Thus up to negligible errors we see that the operator H_{local} is bounded below by

$$\tfrac{1}{2}(2\pi)^{-3} \int -(\mathcal{A}(\vec{k}) + \mathcal{B}(\vec{k})) + \sqrt{(\mathcal{A}(\vec{k}) + \mathcal{B}(\vec{k}))^2 - \mathcal{B}(\vec{k})^2}\, d\vec{k},$$

where

$$\mathcal{A}(\vec{k}) = \mu\ell^3 F_{\ell s(\chi)}(\vec{k}^2) \quad \text{and} \quad \mathcal{B}(\vec{k}) = \nu \widehat{Y}_{\omega/\ell}(\vec{k})$$

with $\nu = \nu_+ + \nu_-$ being the total number of particles in the small box. A fairly simple analysis of the above integral shows that we may to leading order replace $\mathcal{A}$ by $\mu\ell^3\vec{k}^2$ and $\mathcal{B}(\vec{k})$ by $4\pi\nu|\vec{k}|^{-2}$, i.e., we may ignore the cutoffs. The final conclusion is that the local energy is given to leading order by

$$\frac{-1}{2(2\pi)^3} \int 4\pi\nu|\vec{k}|^{-2} + \mu\ell^3|\vec{k}|^2 - \sqrt{(4\pi\nu|\vec{k}|^{-2} + \mu\ell^3|\vec{k}|^2)^2 - (4\pi\nu|\vec{k}|^{-2})^2}\, d\vec{k}$$
$$= -2^{1/2}\pi^{-3/4}\nu \left(\frac{\nu}{\mu\ell^3}\right)^{1/4} \int_0^\infty 1 + x^4 - x^2(2 + x^4)^{1/2}\, dx.$$

If we finally use that

$$\int_0^\infty 1 + x^4 - x^2(2 + x^4)^{1/2}\, dx = \frac{2^{3/4}\sqrt{\pi}\,\Gamma(3/4)}{5\Gamma(5/4)}$$

we see that the local energy to leading order is $-I_0 \nu(\nu/\ell^3)^{1/4}$. For the one-component gas we should set $\nu = \rho\ell^3$ and for the two-component gas we should set $\nu = \phi^2\ell^3$ (see (9.5)). After replacing the sum over boxes by an integral and at the same time replace the discrete Laplacian by a continuum Laplacian, as described above, we arrive at asymptotic lower bounds as in Theorems 9.1 and 9.2.

There is one issue that we have not discussed at all and which played an important role in the treatment of the dilute gas. How do we know

the number of particles in each of the small cubes? For the dilute gas a superadditivity argument was used to show that there was an equipartition of particles among the smaller boxes. Such an argument cannot be used for the charged gas. For the one-component gas one simply minimizes the energy over all possible particle numbers in each little box. It turns out that charge neutrality is essentially required for the energy to be minimized. Since the background charge in each box is fixed this fixes the particle number.

For the two-component there is a-priori nothing that fixes the particle number in each box. More precisely, if we ignored the kinetic energy between the small boxes it would be energetically favorable to put all particles in one small box. It is the kinetic energy between boxes, i.e., the discrete Laplacian term in Theorem 9.5, that prevents this from happening. Thus we could in principle again minimize over all particle numbers and hope to prove the correct particle number dependence (i.e., Foldy's law) in each small box. This is essentially what is done except that boxes with very many or very few particles must be treated somewhat differently from the "good" boxes. In the "bad" boxes we do not prove Foldy's law, but only weaker estimates that are adequate for the argument.

9.5. The Rigorous Upper Bounds.

9.5.1. *The upper bound for the two-component gas.* To prove an upper bound on the energy $E_0^{(2)}(N)$ of the form given in Dyson's formula Theorem 9.2 we shall construct a trial function from the prescription in the Bogolubov approximation. We shall use as an input a minimizer Φ for the variational problem on the right side of (9.4). That minimizers exist can be easily seen using spherical decreasing rearrangements. It is however not important that a minimizer exists. An approximate minimizer would also do for the argument given here. Define $\phi_0(\vec{x}) = N^{3/10}\Phi(N^{1/5}\vec{x})$. Then again $\int \phi_0^2 = 1$. In terms of the unscaled function ϕ in (9.5), $\phi_0(\vec{x}) = N^{-1}\phi(\vec{x})$.

Let ϕ_α, $\alpha = 1, \ldots$ be an orthonormal family of real functions all orthogonal to ϕ_0. We choose these functions below.

We follow Dyson [D2] and choose a trial function which does not have a specified particle number, i.e., a state in the bosonic Fock space.

As our trial many-body wave function we now choose

$$\begin{aligned}\Psi \;=\; & \exp\left(-\lambda_0^2 + \lambda_0 a_{0+}^* + \lambda_0 a_{0-}^*\right) \\ & \times \prod_{\alpha\neq 0}(1-\lambda_\alpha^2)^{1/4} \exp\Big(-\sum_{e,e'=\pm 1}\sum_{\alpha\neq 0}\frac{\lambda_\alpha}{4} e e' a_{\alpha,e}^* a_{\alpha,e'}^*\Big)\,|0\rangle\,, \quad (9.9)\end{aligned}$$

where $a_{\alpha,e}^*$ is the creation of a particle of charge $e = \pm 1$ in the state ϕ_α, $|0\rangle$ is the vacuum state, and the coefficients $\lambda_0, \lambda_1, \ldots$ will be chosen below satisfying $0 < \lambda_\alpha < 1$ for $\alpha \neq 0$.

It is straightforward to check that Ψ is a normalized function.

Dyson used a very similar trial state in [D2], but in his case the exponent was a purely quadratic expression in creation operators, whereas the one used here is only quadratic in the creation operators $a^*_{\alpha e}$, with $\alpha \neq 0$ and linear in $a^*_{0\pm}$. As a consequence our state will be more sharply localized around the mean of the particle number.

In fact, the above trial state is precisely what is suggested by the Bogolubov approximation. To see this note that one has

$$(a_{0\pm} - \lambda_0)\Psi = 0, \quad \text{and} \quad \left(a^*_{\alpha+} - a^*_{\alpha-} + \lambda_\alpha(a_{\alpha+} - a_{\alpha-})\right)\Psi = 0$$

for all $\alpha \neq 0$. Thus the creation operators for the condensed states can be replaced by their expectation values and an adequate quadratic expression in the non-condensed creation and annihilation operators is minimized.

Consider now the operator

$$\gamma = \sum_{\alpha=1}^{\infty} \frac{\lambda_\alpha^2}{1-\lambda_\alpha^2} |\phi_\alpha\rangle\langle\phi_\alpha|. \tag{9.10}$$

A straightforward calculation of the energy expectation in the state Ψ gives that

$$\begin{aligned}\left(\Psi, \sum_{N=0}^{\infty} H_N^{(2)}\Psi\right) &= 2\lambda_0^2\mu \int (\nabla\phi_0)^2 + \mathrm{Tr}\,(-\mu\Delta\gamma) \\ &\quad + 2\lambda_0^2 \mathrm{Tr}\left(\mathcal{K}\left(\gamma - \sqrt{\gamma(\gamma+1)}\right)\right),\end{aligned}$$

where $\mathcal{K}$ is the operator with integral kernel

$$\mathcal{K}(\vec{x},\vec{y}) = \phi_0(\vec{x})|\vec{x}-\vec{y}|^{-1}\phi_0(\vec{y}). \tag{9.11}$$

Moreover, the expected particle number in the state Ψ is $2\lambda_0^2 + \mathrm{Tr}(\gamma)$. In order for Ψ to be well defined by the formula (9.9) we must require this expectation to be finite.

Instead of making explicit choices for the individual functions ϕ_α and the coefficients λ_α, $\alpha \neq 0$ we may equivalently choose the operator γ. In defining γ we use the method of coherent states. Let χ be a non-negative real and smooth function supported in the unit ball in $\mathbb{R}^3$, with $\int \chi^2 = 1$. Let as before $N^{-2/5} \ll \ell \ll N^{-1/5}$ and define $\chi_\ell(\vec{x}) = \ell^{-3/2}\chi(\vec{x}/\ell)$. We choose

$$\gamma = (2\pi)^{-3} \int_{\mathbb{R}^3\times\mathbb{R}^3} f(\vec{u},|\vec{p}|)\mathcal{P}^\perp_{\phi_0}|\theta_{\vec{u},\vec{p}}\rangle\langle\theta_{\vec{u},\vec{p}}|\mathcal{P}^\perp_{\phi_0} d\vec{u}d\vec{p}$$

where $\mathcal{P}^\perp_{\phi_0}$ is the projection orthogonal to ϕ_0,

$$\theta_{\vec{u},\vec{p}}(x) = \exp(i\vec{p}\cdot\vec{x})\chi_\ell(\vec{x}-\vec{u}),$$

and

$$f(\vec{u},|\vec{p}|) = \frac{1}{2}\left(\frac{\vec{p}^4 + 16\pi\lambda_0^2\mu^{-1}\phi_0(\vec{u})^2}{\vec{p}^2\left(\vec{p}^4 + 32\pi\lambda_0^2\mu^{-1}\phi_0(\vec{u})^2\right)^{1/2}} - 1\right).$$

We note that γ is a positive trace class operator, $\gamma\phi_0 = 0$, and that all eigenfunctions of γ may be chosen real. These are precisely the requirements

needed in order for γ to define the orthonormal family ϕ_α and the coefficients λ_α for $\alpha \neq 0$.

We use the following version of the Berezin-Lieb inequality [Be, L3]. Assume that $\xi(t)$ is an *operator* concave function of $\mathbb{R}_+ \cup \{0\}$ with $\xi(0) \geq 0$. Then if Y is a positive semi-definite operator we have

$$\mathrm{Tr}\,(Y\xi(\gamma)) \geq (2\pi)^{-3} \int \xi(f(\vec{u},|\vec{p}|)) \left(\theta_{\vec{u},\vec{p}}, \mathcal{P}_{\phi_0}^{\perp} Y \mathcal{P}_{\phi_0}^{\perp} \theta_{\vec{u},\vec{p}}\right) d\vec{u}d\vec{p}. \qquad (9.12)$$

We use this for the function $\xi(t) = \sqrt{t(t+1)}$. Of course, if ξ is the identity function then (9.12) is an identity. If $Y = I$ then (9.12) holds for all concave ξ with $\xi(0) \geq 0$.

Proving an upper bound on the energy expectation (9.11) is thus reduced to the calculations of explicit integrals. After estimating these integrals one arrives at the leading contribution (for large λ_0)

$$\begin{aligned} 2\lambda_0^2\mu \int (\nabla\phi_0)^2 + \iint & \left(\mu\vec{p}^2 + 2\lambda_0^2\phi_0(\vec{u})^2 \frac{4\pi}{\vec{p}^2}\right) f(\vec{u},|\vec{p}|) \\ & - \frac{4\pi}{\vec{p}^2} 2\lambda_0^2 \phi_0(\vec{u})^2 \sqrt{f(\vec{u},|\vec{p}|)(f(\vec{u},|\vec{p}|)+1)}\; d\vec{p}d\vec{u} \\ = \; & 2\lambda_0^2\mu \int (\nabla\phi_0)^2 - I_0 \int (2\lambda_0^2)^{5/4} \phi_0^{5/2}, \end{aligned}$$

where I_0 is as in Theorem 9.2.

If we choose $\lambda_0 = \sqrt{N/2}$ we get after a simple rescaling that the energy above is $N^{7/5}$ times the right side of (9.4) (recall that Φ was chosen as the minimizer). We also note that the expected number of particles is

$$2\lambda_0^2 + \mathrm{Tr}(\gamma) = N + O(N^{3/5}),$$

as $N \to \infty$.

The only remaining problem is to show how a similar energy could be achieved with a wave function with a fixed number of particles N, i.e., how to show that we really have an upper bound on $E_0^{(2)}(N)$. We indicate this fairly simple argument here.

We construct a trial function Ψ' as above, but with an expected particle number N' chosen appropriately close to, but slightly smaller than N. More precisely, N' will be smaller than N by an appropriate lower order correction. It is easy to see then that the mean deviation of the particle number distribution in the state Ψ' is lower order than N. In fact, it is of order $\sqrt{N'} \sim \sqrt{N}$. Using that we have a good lower bound on the energy $E_0^{(2)}(n)$ for all n and that Ψ' is sharply localized around its mean particle number, we may, without changing the energy expectation significantly, replace Ψ' by a normalized wave function Ψ that only has particle numbers less than N. Since the function $n \mapsto E_0^{(2)}(n)$ is a decreasing function we see that the energy expectation in the state Ψ is, in fact, an upper bound to $E_0^{(2)}(N)$.

9.5.2. *The upper bound for the one-component gas.* The upper bound for the one-component gas is proved in a very similar way as for the two-component gas. We shall simply indicate the main differences here. We will again choose a trial state without a fixed particle number, i.e., a grand canonical trial state. Since we know that the one-component gas has a thermodynamic limit and that there is equivalence of ensembles [LN], it makes no difference whether we choose a canonical or grand-canonical trial state.

For the state ϕ_0 we now choose a normalized function with compact support in Λ, that is constant on the set $\{x \in \Lambda \mid \mathrm{dist}(x, \partial\Lambda) > r\}$. We shall choose $r > 0$ to go to zero as $L \to \infty$. Let us also choose the constant n such that $n\phi_0^2 = \rho$ on the set where ϕ_0 is constant. Then $n \approx \rho L^3$.

Let again ϕ_α, $\alpha = 1, \ldots$ be an orthonormal family of real functions orthogonal to ϕ_0. As our trial state we choose, this time,

$$\Psi = \prod_{\alpha\neq 0}(1-\lambda_\alpha^2)^{1/4}\exp\Big(-\lambda_0^2/2 + \lambda_0 a_0^* - \sum_{\alpha\neq 0}\frac{\lambda_\alpha}{2}a_\alpha^* a_\alpha^*\Big)|0\rangle\,, \quad (9.13)$$

where a_α^* is the creation of a particle in the state ϕ_α. We will choose Ψ implicitly by choosing the operator γ defined as in (9.10).

This time we obtain

$$\begin{aligned}\Big(\Psi, \sum_{N=0}^{\infty} H_N^{(1)}\Psi\Big) &= \lambda_0^2\mu\int(\nabla\phi_0)^2 \\ &+\tfrac{1}{2}\iint\frac{|\gamma(\vec{x},\vec{y})|^2}{|\vec{x}-\vec{y}|}d\vec{x}d\vec{y} + \tfrac{1}{2}\iint\frac{|\sqrt{\gamma(\gamma+1)}(\vec{x},\vec{y})|^2}{|\vec{x}-\vec{y}|}d\vec{x}d\vec{y} \\ &+\tfrac{1}{2}\iint_{\Lambda\times\Lambda}\left(\rho-\rho_\gamma(\vec{x})-\lambda_0^2\phi_0(\vec{x})^2\right)|\vec{x}-\vec{y}|^{-1}\left(\rho-\rho_\gamma(\vec{y})-\lambda_0^2\phi_0(\vec{y})^2\right)d\vec{x}d\vec{y} \\ &+\mathrm{Tr}\left(-\mu\Delta\gamma\right) + \lambda_0^2\mathrm{Tr}\left(\mathcal{K}\left(\gamma-\sqrt{\gamma(\gamma+1)}\right)\right), \end{aligned} \quad (9.14)$$

where $\rho_\gamma(\vec{x}) = \gamma(\vec{x},\vec{x})$ and $\mathcal{K}$ is again given as in (9.11). We must show that we can make choices such that the first four terms on the right side above are lower order than the energy, and can therefore be neglected.

We choose

$$\gamma = \gamma_\varepsilon = (2\pi)^{-3}\int_{|p|>\varepsilon\rho^{1/4}} f(|\vec{p}|)\mathcal{P}_{\phi_0}^{\perp}|\theta_{\vec{p}}\rangle\langle\theta_{\vec{p}}|\mathcal{P}_{\phi_0}^{\perp}d\vec{p},$$

where $\varepsilon > 0$ is a parameter which we will let tend to 0 at the end of the calculation. Here $\mathcal{P}_{\phi_0}^{\perp}$ as before is the projection orthogonal to ϕ_0 and this time

$$f(|\vec{p}|) = \frac{1}{2}\left(\frac{\vec{p}^4 + 8\pi\mu^{-1}\rho}{\vec{p}^2\left(\vec{p}^4 + 16\pi\mu^{-1}\rho\right)^{1/2}} - 1\right)$$

and

$$\theta_{\vec{p}}(x) = \sqrt{n\rho^{-1}}\exp(i\vec{p}\cdot\vec{x})\phi_0(\vec{x}).$$

Note that $n\rho^{-1}\phi_0(\vec{x})^2$ is 1 on most of Λ. We then again have the Berezin-Lieb inequality as before. We also find that

$$\begin{aligned}\rho_\gamma(\vec{x}) &= (2\pi)^{-3}\int_{|p|>\varepsilon\rho^{1/4}} f(|\vec{p}|)d\vec{p}n\rho^{-1}\phi_0(\vec{x})^2\left(1+O(\varepsilon^{-1}\rho^{-1/4}L^{-1})\right)\\ &= A_\varepsilon(\rho/\mu)^{3/4}n\rho^{-1}\phi_0(\vec{x})^2\left(1+O(\varepsilon^{-1}\rho^{-1/4}L^{-1})\right),\end{aligned}$$

where A_ε is an explicit function of ε. We now choose λ_0 such that $\lambda_0^2 = n(1-A_\varepsilon\rho^{-1/4}\mu^{-3/4})$, i.e., such that

$$\lambda_0^2\phi_0^2(\vec{x})+\rho_\gamma(\vec{x}) = n\phi_0(\vec{x})^2(1+O(\varepsilon^{-1}\rho^{-1/2}L^{-1}))\approx\rho.$$

It is easy to see that the first term in (9.14) is of order $\rho L^3(rL)^{-1}$ and the fourth term in (9.14) is of order $\rho L^3(\varepsilon^{-2}+\rho r^2)$. We may choose r, depending on L, in such a way that after dividing by ρL^3 and letting $L\to\infty$ only the error ε^{-2} remains. This allows choosing $\varepsilon \ll \rho^{-1/8}$.

To estimate the second term in (9.14) we use Hardy's inequality to deduce

$$\iint\frac{|\gamma(\vec{x},\vec{y})|^2}{|\vec{x}-\vec{y}|}d\vec{x}d\vec{y}\le 2(\mathrm{Tr}\,\gamma^2)^{1/2}\mathrm{Tr}\,(-\Delta\gamma^2)^{1/2},$$

and these terms can be easily estimated using the Berezin-Lieb inequality in the direction opposite from before, since we are interested now in an upper bound. The third term in (9.14) is controlled in exactly the same way as the second term. We are then left with the last two terms in (9.14). They are treated in exactly the same way as for the two-component gas again using the Berezin-Lieb inequality.

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Exactly Soluble Models

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SOME OF THE EARLY HISTORY OF EXACTLY SOLUBLE MODELS

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The early history of exactly soluble models in statistical mechanics and the quantum-mechanical many-body problem, especially in the 1960's, is briefly reviewed.

Some of the seminal developments in 'exactly soluble models' occurred at Northeastern University in the 1960's, and it was therefore a most fitting location for a workshop on the subject. Since I was involved with some of these developments, the organizers kindly invited me to talk about the early history, especially for those who were not present when it unfolded. I called my talk 'In the beginning...', because my intention was to try to convey some of the atmosphere of statistical mechanics from about 1930 up to about 1970, very roughly speaking. No pretense at historical completeness is made here; this is only a collection of snapshots from the photo album of one who had the pleasure of contributing to the subject in its earliest days. There are bound to be omissions and I ask for the indulgence of many colleagues who should be cited here and are not.

It may be difficult for a young person entering the field now to appreciate the zeitgeist of the 1950's. The big news was *Onsager's solution*[1] *of the two-dimensional Ising model* (with no magnetic field) in 1944. Before that the high point of theoretical equilibrium statistical mechanics was perhaps the Mayer cluster expansion which, although it was a powerful tool for understanding weakly interacting gases, was poorly understood mathematically and physically. It was not known whether the series converged and, if so, whether one could interchange the infinite volume limit with the summation (finally settled by Ginibre, Groeneveld, Lebowitz, Penrose, Ruelle, etc. in the early 1960's).

Concerning the matter of phase transitions, debates raged about whether they could be accounted for in terms of equilibrium statistical mechanics in the Gibbsian formalism (i.e., by computing the partition function and taking the thermodynamic limit). Since the partition function of a finite system is analytic in the temperature, how could the thermodynamic limit be non-analytic? — some said. Of course there were mean field theories, such as the Weiss theory of ferromagnetism, that gave phase transitions, but these did not start from short range forces on an atomic scale.

All this changed with Onsager's remarkable solution. One saw a genuine singularity — and it was not even of the elementary power law type; it was logarithmic!

This became the paradigm of soluble models and the paradigm of phase transitions. Although today we regard the solution as relatively easy (it is 'merely' a free fermion theory, is it not?) it was not so regarded until perhaps the mid 60's — and then only by a relatively small number of afficionados. It may be difficult for today's experts, of which there are many, to appreciate the mystique that surrounded Onsager's solution. Hyperbolically speaking, it was in the same league as Einstein's theory of general relativity, about which the popular press once said that only a handful of physicists were capable of understanding it. The calculation, which used the transfer matrix method had to be simplified and this was done, first of all, by Kaufmann's spinor analysis,[2] and later by Schultz-Mattis-Lieb[3] who introduced the Jordan-Wigner transformation into the statistical mechanics of quantum spin chains and two-dimensional lattice problems.

It is truly amazing how alive this model is today. One would have thought that its solution would end the story, but much remained to be discovered in the way of correlation functions, etc.. Abraham, for instance, still continues to deduce interesting physics from this model by ingenious choices of boundary and other conditions (see Ref.[26]). A grail (perhaps not a holy one) is to solve the problem with an external magnetic field, but that has eluded us. However, Onsager and Yang[4] did manage, by independent, but equally impressive means, to find the spontaneous magnetization of this model. It was not until fairly late, however, that Aizenman[5] and Higuchi[6] managed to prove that there is never any phase coexistence in this model (because it is two-dimensional).

Subsequently there were several solutions to the two-dimensional Ising model that did not use the transfer matrix, but special mention has to be made of the solution in which the problem is first mapped into a dimer covering problem on a slightly more complicated lattice. The dimer problem was solved by Temperley-Fisher[7] and Kasteleyn[8] (whose death just a few months before the workshop saddened us greatly). Kasteleyn found out how to treat the most general planar graph, and I cannot resist going outside my stated time frame and mentioning that the cleanest and simplest derivation of Kasteleyn's general theorem is now probably the one of Loss and me.[9] The dimer problem has a life of its own and has found many applications, not only in statistical mechanics (where, in particular, it yields another solution of Onsager's problem) but also in combinatorial theory.

There were, of course, other soluble models that had been invented, mostly in one-dimension, and summarized in my book with Mattis.[10] None, however, had the impact of the Ising model because none had the feature of proving that a phase transition can result from short range forces. [Parenthetically, one might mention a totally different line of attack in which phase transitions can be proved to occur without actually obtaining a closed form solution. This has been very fruitful because the number of models that can be treated this way vastly exceeds the number of exactly soluble ones. The main techniques involve either the 'Peierls argument', pioneered by Dobrushin (who also died just a few months ago, leaving us a legacy of superb contributions to mathematical physics) and Griffiths, or reflection

positivity and infrared bounds; I will not discuss them here because they fall outside the topic of exact solubility.]

Many models are mentioned in our book, and I can not attempt to discuss them all. One that I am fond of, and which has not had quite the notoriety it deserves, is the solution of the one-dimensional, two-component Coulomb gas, discovered simultaneously by Lenard and Prager; shortly thereafter Baxter did the same thing for the one-component jellium model (see Ref.[10]). What is striking about this, apart from the mathematical beauty of the solution, is the following: There is a simple 'physical' theory of the weak coupling regime—the Debye-Hückel theory—that is asymptotically exact in the limit of zero coupling. On the other hand, the exact solution (which involves the solution to Mathieu's equation) is simple in the strong coupling regime but extremely difficult in the weak coupling regime. Another example of this phenomenon is the delta-function gas mentioned below; the Bogoliubov theory is simple and exact in the limit of weak coupling but the exact solution is difficult to analyze in this limit. In short, a 'physical' perturbation is sometimes a singular perturbation, mathematically speaking, and hence difficult to analyze rigorously.

Among the exactly soluble models was one that for a long time was a 'sleeper', namely Bethe's 1931 solution[11] of the ground state energy and the elementary excitations of the one-dimensional quantum-mechanical spin-1/2 Heisenberg model of antiferromagnetism. This quantum mechanical model appeared to have nothing to do with statistical mechanics and was regarded as every bit as mysterious as the Onsager solution, except that much less attention was paid to it because it was one-dimensional. One person who understood it well was Hulthén who actually calculated the ground state energy[12] in 1938, and whose contribution to the subject seems, alas, to have been mostly overlooked. The extraction of meaningful information from Bethe's solution was taken up again by Yang and Yang in a 1966 paper[13] noteworthy for its elegant analysis; these results were very important in connection with the solution of the 6-vertex models to be mentioned later.

In some sense the 'natural' setting for Bethe's ansatz is the continuum (line segment) rather than the lattice because some of the technicalities simplify there. In 1963 Liniger and I[14] investigated the Bose gas of particles interacting via repulsive delta-functions. At that time the problem of interpreting the superfluidity of liquid helium in terms of a Bose-Einstein condensation was a popular topic, and that was our motivation. With the recent direct experimental observation of Bose-Einstein condensation for weakly interacting cold atoms the subject has a new lease on life. Alas, many of the old theoretical puzzles have still not been straightened out—to my taste, at least. The Bose-Einstein condensate (if it is not zero) is not the same as the superfluid fraction (at $T = 0$ the former is perhaps a few percent while the latter is 100%) and the relation between the two quantities needs clarification.

An interesting point about this exact one-dimensional solution was that the Bogoliubov approximation for the ground state energy turned out to be excellent at weak coupling in many respects (it is exact in the limit)—despite the fact that it is

predicated on the existence of a condensate which is surely absent in one-dimension. One way in which the Bogoliubov theory turned out to be inadequate was that there are two elementary excitation modes, not one as the Bogoliubov theory predicts.

Independently of our work on the repulsive delta-function gas, McGuire worked out the exact many-body scattering theory of delta-function bosons[15] and he found the ground state for the attractive delta-function (which is a bound state) but which, unfortunately, does not have a nice thermodynamic limit unless the coupling constant is tuned to the density. Yang and Yang figured out how to compute the thermodynamics of the repulsive delta-function gas[16] exactly, but it took 24 years until Dorlas, Lewis and Pulé constructed a proof of this remarkable construction.[17]

At this point in the story it might be worth mentioning that most of the early work was motivated by physics and that writing down a formal solution was regarded as only part of the exercise. Much effort went into figuring out the physical consequences, to the extent possible, of an exact solution. Sometimes it seems that this motivation receded into the background as the subject evolved, and I consider this a pity. More and more the emphasis has shifted to finding the mathematical structure of solutions and people seem to be content with formal solutions. While mathematical structure is important and aesthetically pleasing, it is not a substitute for physics. Without strong roots in physics this field will have to be judged purely as mathematics, and from that point of view it might not have the importance it has.

With the realization that there were many papers on exactly soluble models and other rigorous results in one-dimension—in many areas of physics—Mattis and I decided to put them together in a reprint volume with extensive commentary[10] in 1965. The exercise took two years and was harder than we thought, but it was worth it. We learned a lot, at least, and so did others. One of the fruits of our effort was the realization that Luttinger's solution of his version of Tomonaga's model of interacting electrons was not right. The Bethe ansatz was not appropriate in this case and our correct solution required the invention of an idea[18] that eventually turned out to be useful in other contexts as well, namely, 'bosonization'. Subsequently, there were 'solutions' to more complicated versions of the model, but it is not entirely clear which ones are entirely free of similar problems. It seems that some of the later problem solvers did not think it worthy of a physicist's time to try to worry about rigor. While this attitude may be generally reasonable, the history of this particular problem shows that danger lurks in such an attitude. Exactly soluble models that are not exactly solved can be an impediment to understanding. It should be a goal to keep the literature in this subfield as clean and unambiguous as possible.

It might be difficult for today's model solvers to appreciate the fact that most physicists then considered work on one-dimension to be an unadulterated waste of time. It 'clearly' had nothing to do with physics and, moreover, was an exercise in mathematics for its own sake which, as everyone knew, was some kind of siren's call toward which one's ears had to be sealed. Fortunately, we now know better, at

least as far as the reality of one-dimensional physics goes. The attitude toward the role of mathematics in physical thinking has also improved, but perhaps not yet as much as it ought. In any case, the book was important because it established a field that was not recognizable before, and which continues to flourish.

In this vein, it is useful and comforting to note that there can be a reversal of roles between what is currently considered to be 'frontline' and what is considered to be 'back-water'. Sometimes old and/or peculiar things can become popular (such as exactly soluble one-dimensional models) or revive their previous glory (such as mechanics, quantum measurement theory, or maybe eventually even classical thermodynamics).

1966 was the year I came to Northeastern University and happily joined the group of young physicists who were building up a significant physics department. One of the problems I attacked (thanks to the inspiration of Nagle) was the exact enumeration of Pauling's ice model configurations on a two-dimensional square lattice. Nagle had calculated it numerically in two- and three-dimensions, which now seems easy to do but which required considerable cleverness given the available computing power at that time. I was able to see that Bethe's ansatz, originally invented for the one-dimensional spin system, could solve the transfer matrix problem of this two-dimensional system—also known as the six-vertex model. Asymptotically, the number of configurations for an N atom crystal of 'square ice' turned out to be[19]

$$\left(\frac{4}{3}\right)^{\frac{3}{2}N} . \tag{1}$$

(By the way, Pauling's explanation of the residual entropy of ice is one of the most accurate calculations about real, strongly interacting matter in all of statistical mechanics. Unfortunately, it is not as widely known as it should be. Apart from a few examples like this, statistical mechanics is more a paradigm of a qualitative theory than a quantifiable one.)

Next came the antiferroelectric six-vertex F-model[20] of Fierz and Rys, which introduced some nontrivial parameters, and hence a phase transition, into the game. Then Slater's KDP model[21] of a ferroelectric. Oddly, the F model has an infinite order phase transition (quite different from Onsager's Ising model) while the KDP model has a first order transition. All the possible combinations of the two models were solved by Sutherland.[22] These models could be solved with an external electric field parallel to one lattice direction (again, different from Onsager's model). Moreover, Sutherland, Yang and Yang were able to solve the model with a field[23] in an arbitrary direction, thereby bringing the number of nontrivial pararameters of the six-vertex model to four—which exceeds the number (three) of the parameters for which the eight-vertex model can be solved. (It would be desirable to have a rigorous verification of the assumption in Ref.[23] that in the thermodynamic limit the k's lie on a smooth curve with a nice density.) Some interesting special cases were worked out by Wu who moved to Northeastern University in 1967. Together, we incorporated everything known about these six-vertex models into a review article.[24]

Important contributions to the article were also made by Abraham, Barouch, Baxter and Glasser. Indeed, it was not easy to work out many intricate, but interesting details. An example is the analyticity in the temperature for the F-model; not only does this model have an infinite order phase transition, it also has a natural boundary in the complex plane—a phenomenon that is mathematically 'generic' but which is usually discounted in physics speculations.

The six-vertex model later had several physical manifestations besides ice. For instance there is the solid-on-solid model of van Beijern,[25] the facet formation model of Abraham,[26] domain walls, and the model of sodium trihydrogen selenite.[27] One theoretical spin-off that turned out to have interesting consequences for knot theory was the Temperley-Lieb algebra[28] which grew out of a method of representing the transfer matrix for a percolation problem by doubling the number of sites on each line of a square lattice.

Another very important offshoot was, of course, Baxter's solution of the eight-vertex model,[29] which was a marvelous example of mathematical virtuosity, and which opened a new chapter in the subject. That takes us into the 70's, however, and I will refer the reader to Baxter's account in his lecture in this workshop.

As a last topic about exact solutions in the 60's, let me mention the many-fermion problem. The delta-function Bose gas was solved with an ansatz of the Bethe type. Could a modified version of this ansatz also work for N spin-1/2 fermions? When one spin is down and $N-1$ are up the problem was solved by McGuire,[30] but the full complication is not seen until two spins are reversed. This was done by Flicker and me,[31] but a short while later Gaudin[32] did the general case in his Ph.D. thesis (quite independently). Yang also found the solution.[33] Wu and I then realized that the lattice version of this model—the Gutzwiller-Hubbard-Kanamori model (but which was known much earlier in the chemistry literature as the Pariser-Parr-Pople model)—could be solved the same way,[34] thus completing the circuit from Bethe's lattice spin model, through the continuum Bose gas, to the lattice model of interacting fermions. Ovchinnikov[35] then worked out the spectrum of elementary excitations. This exact solution had several interesting consequences, one of which is that it acted as a touchstone for approximation schemes in the difficult area of 'electron correlations', especially in the era of high T_c superconductivity. Another point is the double excitation spectrum (called 'holons and spinons' by Anderson), which some people believe is also qualitatively valid in two-dimensional systems. (It is certainly present in the one-dimensional Bose gas.[14]) In any case, I am told that photoemission experiments are now beginning to see this double spectrum.

All of which goes to show that the exactly soluble models have an interesting, physically relevant, and apparently enduring life of their own.

Acknowledgements

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Part IX

The Six-Vertex Ice Type Models

Phys. Rev. Lett. *18*, 692–694 (1967)

VOLUME 18, NUMBER 17 PHYSICAL REVIEW LETTERS 24 APRIL 1967

EXACT SOLUTION OF THE PROBLEM OF THE ENTROPY OF TWO-DIMENSIONAL ICE

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The entropy of two-dimensional ice has been found by the transfer-matrix method. Entropy $= Mk \ln W$, with $M =$ No. of molecules and $W = (\frac{4}{3})^{3/2}$.

At low temperatures ice has a residual entropy caused, presumably, by an indeterminacy of the crystal structure. The oxygen atoms constitute a periodic crystal lattice that is hydrogen bonded. The hydrogen atoms are not at the centers of the bonds, however, so that there are two possible states for each bond corresponding to the two positions of the hydrogen atom relative to the bond midpoint. Nevertheless, not all bond configurations are allowed, for there is a constraint called the "ice condition" such that for the four bonds emanating from each oxygen atom, exactly two of the bonds must have the hydrogen atoms close to the oxygen atom.

This problem has received a good deal of theoretical and numerical attention,[1-6] and the best numerical estimates of the entropy are in excellent agreement with experiment.[6] While the problem has also attracted the attention of math-

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ematicians, no exact analytic solution of the problem has heretofore been obtained.

We have succeeded in solving the two-dimensional version of the problem which may be formulated as follows: Let the vertices of a square $N\times N$ net (as in the Ising model) represent the oxygen atoms, and on each bond draw an arrow (up or down for vertical bonds and left or right for horizontal bonds). The "ice condition" is that there must be precisely two arrows into each vertex. If $M=N^2$, then for large M the number of arrangements will be W^M, where W is to be calculated. The entropy is $Mk\ln W$. If we ignore the "ice condition," then obviously $W=4$.

The best numerical estimate[6] for W in two dimensions was $W=1.540\pm 0.001$. Our exact result is

$$W=(\tfrac{4}{3})^{3/2}=1.539\,600\,7.$$

The calculation uses the well-known transfer-matrix formalism which we briefly outline here. A configuration of the lattice consists of N rows of N vertical arrows alternating with N rows of N horizontal arrows. Let φ^1 represent a definite configuration of the first "vertical" row. There are obviously 2^N choices for φ^1. Likewise, let φ^j be the configuration of the jth "vertical" row. If φ and φ' are the configurations of two successive "vertical" rows, let $A(\varphi,\varphi')$ be the number of ways of placing arrows on the intervening "horizontal" row such that the ice condition is satisfied at every vertex of that "horizontal" row. Thus, A is a 2^N square matrix whose entries are integers, and Z, the total number of ways of correctly placing arrows on the lattice, is then $Z=\mathrm{Tr}A^N$ (assuming the lattice to be wrapped on a torus). As usual, $Z=\lambda^N$, where λ is the largest eigenvalue of A.

In general, a state φ' differs from φ by the replacement of certain "up" arrows by "down" arrows, namely, a +− exchange, or the reverse, which is a −+ exchange. A little reflection yields the following matrix elements for $A(\varphi,\varphi')$: (i) $A(\varphi,\varphi)=2$; (ii) for $\varphi\neq\varphi'$, $A(\varphi,\varphi')=1$ if there is a +− exchange between every pair of −+ exchanges, and vice versa; and (iii) $A(\varphi,\varphi')=0$, otherwise. If we regard a state φ as a state of N spin-$\frac{1}{2}$ particles on a line, then the above rule is equivalent to $A=A_L+A_R$, where

$$A_L=1+\sum_{i<j}S_i^-S_j^+ +\sum_{i<j<k<l}S_i^-S_j^+S_k^-S_l^+ +\cdots+(S_1^-S_2^+\cdots S_{N-1}^-S_N^+)$$

(assuming N is even) and $A_R=A_L^+$. Since $S^z=\sum_1^N S_i^z$ is a constant, we must decide which S^z subspace has the largest eigenvalue. It can be shown, as expected, that $S^z=0$ has the largest.

If ψ is an eigenvector of A, let $f(x_1,\cdots,x_n)$ be the amplitude in ψ of the state with up arrows (spins) at the sites $x_1<x_2<\cdots<x_n$ (we are interested in $n=\frac{1}{2}N$). Further reflection shows that f satisfies

$$\lambda f(x_1,\cdots,x_n)=\sum_{y_1=1}^{x_1}\sum_{y_2=x_1}^{x_2}\cdots\sum_{y_n=x_{n-1}}^{x_n}f(y_1,\cdots,y_n)+\sum_{y_1=x_1}^{x_2}\sum_{y_2=x_2}^{x_3}\cdots\sum_{y_n=x_n}^{N}f(y_1,\cdots,y_n). \quad (1)$$

On the right-hand side of (1) it is to be understood that f is replaced by zero if any $y_i=y_{i+1}$ (e.g., $y_2=y_1=x_1$).

We make the following Ansatz for f: Let $\{k\}=k_1,\cdots,k_n$ be a set of distinct numbers and let

$$f(x_1,\cdots,x_n)=\sum_P{}'A(P)\exp\{i\sum_{i=1}^{n}k_{P(i)}x_i\}, \quad (2)$$

where the sum is on $n!$ permutations and $A(P)$ is some set of $n!$ coefficients. Now, if we insert a given plane wave $\exp\{i\sum k_i x_i\}$ into the first sum in (1), we get (assuming no $k_i=0$)

$$\{\Pi_j[1-\exp(ik_j)]^{-1}\}[e^{ik_1}-e^{ik_1(x_1+1)}][e^{ik_2x_1}-e^{ik_2(x_2+1)}]\cdots\{\exp[ik_nx_{n-1}]-\exp[ik_n(x_n+1)]\}. \quad (3)$$

Expanding the above product gives 2^n terms. One of these is proportional to the same plane wave we started with and is desirable. All the others are unwanted because one or more x_i's fail to appear.

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The situation is saved, however, because we are obliged to subtract from (3) those terms in (1) for which $y_i = y_{i+1} = x_i$, and these have the same character as the unwanted terms. A similar situation obtains for the second sum in (1).

By choosing the $A(P)$ correctly we can eliminate all the unwanted terms. The rule (which can be proved by induction) is this: If P and Q are two permutations which differ only in the jth and $(j+1)$th position, then

$$A(P) = A(Q)B(k, q), \tag{4}$$

where $k_{P(j)} = k_{Q(j+1)} = k$ and $k_{P(j+1)} = k_{Q(j)} = q$, and where

$$B(k, q) = -[1 + T(k)T(q) - T(k)][1 + T(k)T(q) - T(q)]^{-1}$$

with $T(k) = \exp(ik)$. Finally, periodicity comes in through the n conditions

$$\exp(ik_i n) = \prod_{j \neq i} B(k_i, k_j). \tag{5}$$

The eigenvalue, λ, is the coefficient of the wanted term from A_L and A_R, namely,

$$\lambda = \{\prod_{j=1}^{n} (1 - \exp ik_j)^{-1}\}\{1 + \exp(i\sum_{1}^{n} k_j)\}. \tag{6}$$

It will be recognized that our wave function as defined by (4) and (5) is exactly the same as that for the anisotropic one-dimensional Heisenberg model[7]:

$$H = -\sum_{i=1}^{N} S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \tfrac{1}{2} S_i^z S_{i+1}^z. \tag{7}$$

Our eigenvalue (6) is different, however. For n even, the solution to (5) is such that no $k = 0$ and thus our previous analysis is correct. Furthermore, the maximum eigenstate of the transfer matrix and the ground state of (7) are identical because both are characterized by the fact that $f(x_1, \cdots, x_n) > 0$. For this state,

$$\sum_{j=1}^{n} k_j = 0.$$

As $N \to \infty$ one introduces a density function $\rho(k)$ for the k's. This function satisfies an integral equation which, fortunately, can be solved exactly for $S^z = 0$. All the details are in Ref. 7 where it is shown that in terms of a new variable α defined by $e^{ik} = (e^{i\mu} - e^{\alpha})(e^{i\mu + \alpha} - 1)^{-1}$ (with $\cos\mu = -\frac{1}{2}$), the density function is given by $R(\alpha) = [4\mu \cosh(\pi\alpha/2\mu)]^{-1}$.

Thus, we have

$$N^{-1} 2 \ln\lambda = -\int dk\, \rho(k) \ln(2 - 2\cos k),$$

$$= -\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{3 d\alpha}{4\cosh(3\alpha/4)} \ln\left(1 - \frac{3}{1 + 2\cosh\alpha}\right)$$

$$= 3\ln(\tfrac{4}{3}).$$

Therefore, $W = \lambda^{1/N} = (\frac{4}{3})^{3/2}$.

I should like to thank Professor S. Sherman and Dr. J. Nagle for introducing me to the problem.

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EXACT SOLUTION OF THE *F* MODEL OF AN ANTIFERROELECTRIC

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The Rys *F* model of an antiferroelectric is solved by the transfer-matrix method. The result is different in many respects from the analogous Ising antiferromagnet, i.e., an infinite-order phase transition and a natural boundary in the complex T plane. It can also be solved when an external electric field is included. Above the transition temperature the behavior is normal while below T_C there is no polarization unless the electric field is sufficiently large.

The *F* model, which was originally proposed by Rys[1] as an interesting statistical mechanics problem, has since[2] become a meaningful model of hydrogen bonded ferroelectrics (e.g., $NH_4H_2PO_4$), at least in the sense that the two-dimensional Ising model is a reasonable model for an antiferromagnet. We have succeeded in solving this model by an extension of the method used to find the residual entropy of square ice.[3]

The solution has several unusual features:

(1) The free energy has a branch point at the critical temperature (as usual), but the cut is a natural boundary instead of a movable cut (e.g., $\ln|T-T_C|$).

(2) The phase transition is infinite order, i.e., the free energy and all its derivatives are finite and continuous at T_C. The free energy has an asymptotic power series about T_C with a zero radius of convergence. In particular, there is no latent heat.[2]

(3) Unlike the Ising model, the *F* model can be solved when an external electric field $\mathcal{E}$ is included (we wish to thank Professor J. Lebowitz for suggesting we treat the application of an electric field). For $T>T_C$, the polarization versus $\mathcal{E}$ is the usual S-shaped curve, saturating at $\mathcal{E}=\infty$. For $T<T_C$, however, the polarization is 0 for $\mathcal{E}<\mathcal{E}_C$ (where $\mathcal{E}_C$ depends on T). For $\mathcal{E}>\mathcal{E}_C$, the polarization behaves normally. The Ising antiferromagnet does not have this property.

The statement of the problem is the following: Place arrows on the bonds of a square $N\times N$ lattice and allow only those configurations with precisely two arrows pointing into each vertex. (Thus far we have the ice problem.) Next, we assign energies to the six kinds of vertices (Fig. 1): $e_1=e_2=e_3=e_4=\epsilon>0$, $e_5=e_6=0$. If, in addition, we apply an electric field $\mathcal{E}$ in the vertical direction, there is an additional energy $-\mathcal{E}d(N^2-2n)$, where d is the dipole moment and $2n$ is the number of downward vertical arrows. The partition function is

$$Z=\sum\exp[-Km+E(N^2-2n)], \tag{1}$$

where the sum is over allowed configurations; $E=\mathcal{E}d/kT$, $K=\epsilon/kT$, and m is the number of types 1, 2, 3, and 4 vertices.

Let φ and φ' be the configurations of two successive rows of vertical bonds and introduce the transfer matrix

$$A(\varphi,\varphi')=\sum\exp(-Km), \tag{2}$$

where m is now the number of types 1, 2, 3,

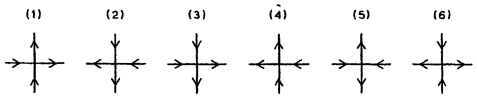

FIG. 1. The six kinds of vertex configurations allowed by the "ice condition." The associated energies for the *F* model are $e_1=e_2=e_3=e_4=\epsilon>0$; $e_5=e_6=0$. From F. Y. Wu, Phys. Rev. Letters 18, 605 (1967).

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and 4 on the single row of vertices and where the sum is now over allowed arrangements of intervening horizontal arrows. If n is the number of downward vertical arrows in φ then A is replaced by $A' = \exp[E(N-2n)]A(\varphi, \varphi')$ with an electric field. Thus, $Z = \mathrm{Tr}[A'^N] =$ (largest eigenvalue)^N. As we showed previously,[3] A conserves the number n. Let $y = 1-2n/N$ and let $\Lambda_N(y)$ be the largest eignevalue of A in any given n subspace. Then

$$Z = \max_y [\Lambda_N(y)]^N \exp[N^2 E y]. \tag{3}$$

Let $f(x_1, \cdots, x_n)$ be the amplitude in some eigenvector for having downward vertical arrows at sites $x_1, \cdots, x_n$. The eigenvalue equation is similar to the ice problem[3]:

$$\Lambda f(x_1, \cdots, x_n) = \left(\sum_{y_1=1}^{x_1} \cdots \sum_{y_n=x_{n-1}}^{x_n} + \sum_{y_1=x_1}^{x_2} \cdots \sum_{y_n=x_n}^{N} \right) \times f(y_1, \cdots, y_n) D(X, Y), \tag{4}$$

where

$$D = \exp\left[-NKy - 2K \sum_{i,j=1}^{n} \delta(x_i - y_j)\right]$$

Again, the plane-wave Ansatz works:

$$f(x_1, \cdots, x_n) = \sum_P{}' a(P) \exp\left[i \sum_{j=1}^{n} k_{P(j)} x_j\right], \tag{5}$$

and we find (for n even) the following: (1) If $P = \cdots p, q, \cdots$ and $Q = \cdots q, p, \cdots$ then $a(P) = a(Q)B(p,q)$ with $B(p,q) = -[1+T(p)T(q) - 2\Delta T(p)] \times [1+T(p)T(q) - 2\Delta T(q)]^{-1}$, where $\Delta = 1 - \frac{1}{2}\exp(2K)$ and $T(p) = \exp(ip)$; (2) for all $i = 1, \cdots, n$,

$$\exp(ik_i N) = \prod_{j \neq i} B(k_i, k_j);$$

and (3)

$$\Lambda = \prod_j \{e^{-2K} - (1 - e^{ikj})^{-1}\} + \prod_j \{e^{-2K} - (1 - e^{-ikj})^{-1}\}. \tag{6}$$

It will be recognized that we have constructed the eigenvectors of the Heisenberg chain

$$H = -\sum_1^N S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z, \tag{7}$$

although with different eigenvalues. The maximum Λ corresponds to the ground state of (7) because both are positive.

The properties of the set $\{k\}$ for the ground state of (7) are well understood and we quote the results[4]: (1) For each k, there is a $-k$. (2) For large N, the k's are distributed between $-Q$ and Q (which depends on y) with a distribution function $\rho(k)$. (3) It is convenient to change variables to $e^{ik} = (e^{i\mu} - e^{\alpha})(e^{i\mu} + \alpha - 1)^{-1}$ for $\Delta > -1$, with $\Delta = -\cos\mu$, and to $e^{ik} = (e^{\lambda} - e^{-i\alpha}) \times (e^{\lambda - i\alpha} - 1)^{-1}$ for $\Delta < -1$, with $\Delta = -\cosh\lambda$. The critical point is thus $\Delta = -1$ corresponding to a critical temperature $e^K = 2$. (4) In the new variables we introduce $R(\alpha)$ [such that $R(\alpha)d\alpha = 2\pi\rho(k)dk$] in terms of which

$$N^{-2}\ln Z(y) = N^{-2}\ln\Lambda_N(y) + Ey \equiv f(y) = -\frac{1}{4\pi}\int_{-b}^{b} R(\alpha)C(\alpha)d\alpha + Ey - K, \tag{8}$$

and free energy per vertex $= -kT\max_y f(y)$;

$$C(\alpha) = \ln[(\cosh\alpha - \cos 2\mu)/(\cosh\alpha - 1)], \quad \Delta > -1: = \ln[(\cosh 2\lambda - \cos\alpha)/(1 - \cos\alpha)], \quad \Delta < -1. \tag{9}$$

The distribution R and the limit b are determined by the integral equation

$$R(\alpha) = \xi(\alpha) - \int_{-b}^{b} K(\alpha - \beta)R(\beta)d\beta, \tag{10}$$

$$\pi(1-y) = \int_{-b}^{b} R(\alpha)d\alpha, \tag{11}$$

where

$$\xi(\alpha) = \sin\mu[\cosh\alpha - \cos\mu]^{-1}, \quad \Delta > -1, = \sinh\lambda[\cosh\lambda - \cos\alpha]^{-1}, \quad \Delta < -1; \tag{12}$$

$$K(\alpha) = (2\pi)^{-1}(\sin 2\mu)[\cos\alpha - \cos 2\mu]^{-1}, \quad \Delta > -1, = (2\pi)^{-1}(\sinh 2\lambda)[\cosh 2\lambda - \cos\alpha]^{-1}, \quad \Delta < -1. \tag{13}$$

When $y = 0$, $b = \infty$ for $\Delta > -1$ and $b = \pi$ for $\Delta < -1$. Equation (10) may then be solved by Fourier transforms:

$$R(\alpha) = \pi[2\mu\cosh(\pi\alpha/2\mu)]^{-1}, \quad \Delta > -1, = (\pi/2\lambda)\sum_{n=-\infty}^{\infty} \mathrm{sech}[\pi(\alpha + 2\pi n)/2\lambda], \quad \Delta < -1. \tag{14}$$

Now, it can be shown on general grounds that,

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as $N\to\infty$, $N^{-2}\ln\Lambda_N(y)$ is a continuous concave, symmetric function of y. Hence, for $E=0$ the optimum choice is $y=0$. The free energy is obtained by inserting (14) and (9) into (8). The resulting function of temperature has a cut which is a natural boundary and we shall discuss its properties elsewhere. When the second form of (14) and (9) is inserted into (8) the integral can be done explicitly term by term and we thus obtain the following expression for $\delta=0$ and $\Delta<-1$:

$$N^{-2}\ln Z=\tfrac{1}{2}\lambda-K+\tfrac{1}{2}\sum_{n=1}^{\infty}(1-e^{-2n\lambda})(n\cosh n\lambda)^{-1}. \quad (15)$$

For small μ or λ (i.e., $T\sim T_c$), the free energy has an asymptotic, divergent power series which is the same above and below T_c. In terms of μ it is

$$N^{-2}\ln Z=-K+2\ln[\Gamma(\tfrac{1}{4})/2\Gamma(\tfrac{3}{4})]+\tfrac{1}{2}\sum_{n=1}^{\infty}\frac{B_{2n}\mu^{2n}}{n(2n)!}[(-1)^n-|E_{2n}|]. \quad (16)$$

If we differentiate (16) with respect to μ, we find at T_c

$$\text{Energy/vertex}=\tfrac{1}{3}\epsilon,$$

$$\text{Specific heat/vertex}=k(\ln 2)^2(28/45). \quad (17)$$

By virtue of the concavity mentioned above, as E increases y increases continuously. For small y one does perturbation theory on (10) and (11). b decreases with increasing y. For $\Delta>-1$, $b\approx\infty$ so that $N^{-2}\ln[Z(y)/Z(0)]\approx Ey-\text{const}\times y^2$ and the polarization ($=N^2y$) is proportional to E. For $\Delta<-1$, b is finite ($\approx\pi$) and $N^{-2}\times\ln[Z(y)/Z(0)]\sim Ey-\text{const}\times y$. Hence, there is no polarization unless E is large enough.

For $y\approx 1$, on the other hand, (10) and (11) are simple because $b\approx 0$. Thus $b\approx\pi(1-y)\times[2\xi(0)]^{-1}$. When this is inserted into (8) one finds $N^{-2}\ln Z\approx -K+Ey+s(1-y)+t(1-y)\ln(1-y)$, with s and t constants. Hence, for large E, the polarization is

$$y\approx 1-(2/\pi)\exp(-2E+2K). \quad (18)$$

This result is in marked contrast to the analogous magnetization of the Heisenberg chain which, in the ground state, saturates with a finite magnetic field. The difference is a consequence of the logarithmic divergence of (9) at $\alpha=0$.

Dr. F. Y. Wu has kindly informed me (private communication) that he has evaluated the partition function by the dimer method for the particular case $\Delta=0$ ($e^K=\sqrt{2}$ or $\mu=\frac{1}{2}\pi$), but for all y. Indeed, when $\Delta=0$, $K(\alpha)=0$ so that $R(\alpha)=\xi(\alpha)=(\cosh\alpha)^{-1}$ and $\sinh b=\tan\frac{1}{2}\pi(1-y)$. If we insert this result into (8) and change variables to $(\cosh\alpha)^{-1}=\cos k$ we obtain

$$N^{-2}\ln Z(y)=Ey-\tfrac{1}{2}\ln 2+\frac{1}{4\pi}\int_{-Q}^{Q}dk\,\ln\frac{1+\cos k}{1-\cos k}, \quad (19)$$

where $Q=\frac{1}{2}\pi(1-y)$. The integral in (19) can be evaluated for $y=0$, whence

$$N^{-2}\ln Z(0)=-\tfrac{1}{2}\ln 2+(2/\pi)(\text{Catalan's constant})=0.236\,548\,2. \quad (20)$$

I should like to thank Dr. A. Y. Sakakura for a useful conversation.

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EXACT SOLUTION OF THE TWO-DIMENSIONAL SLATER KDP MODEL OF A FERROELECTRIC

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The Slater KDP model is solved for all temperatures and with an electric field. Above T_c the specific heat behaves like $(T-T_c)^{-1/2}$ and the polarizability like $(T-T_c)^{-1}$. There is a first-order phase transition at T_c (latent heat). Below T_c the free energy is simply $-|\mathcal{E}|d$ ($\mathcal{E}$ = electric field, d = dipole moment).

Slater[1] introduced a model of hydrogen-bonded ferroelectrics known as the KDP model, since it was supposed to account for KH_2PO_4 and similar substances. He treated the model by mean field theory and obtained a first-order phase transition (latent heat). The position of the critical temperature T_c and the value of the latent heat were shown to be correct by Takahashi.[2] The model has been widely discussed.[3]

Recently, Wu[4] gave an exact treatment of a modified version of the two-dimensional Slater model. He obtained the same T_c as Slater but found a second-order phase transition (no latent heat). Wu also found that the specific heat C was 0 for all $T < T_c$ and $C \sim (T-T_c)^{-1/2}$ near and above T_c. This contrasts with Slater's result that C is finite at T_c.

In this paper we give an exact solution of the original Slater model in two dimensions. We also wish to emphasize that the analysis is somewhat different above and below T_c and that we have solved the model in both temperature ranges. Our results are the following: (1) Below T_c, $C = 0$ as found by Wu. (2) There is a latent heat at T_c which agrees with Slater's value. (3) $C \sim (T-T_c)^{-1/2}$ near and above T_c, which agrees with Wu. (4) Near and above T_c the polarizability goes like $(T-T_c)^{-1}$, which agrees with Slater's treatment (Wu did not discuss the polarizability of his model).

The mathematical statement of the problem is to place arrows on the bonds of a square $N \times N$ net so that precisely two arrows point into each vertex. Associated with the six allowed vertices (Fig. 1) are energies $e_1 = e_2 = 0$, $e_3 = e_4 = e_5 = e_6 = \epsilon > 0$. In the F model of an antiferroelectric discussed previously,[5] the assignments were $e_1 = e_2 = e_3 = e_4 = \epsilon > 0$, $e_5 = e_6 = 0$.

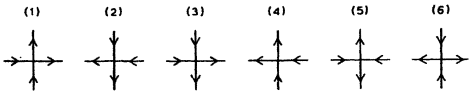

FIG. 1. The six allowed vertex configurations for the Slater KDP model in two dimensions. The energies are $e_1 = e_2 = 0$; $e_3 = e_4 = e_5 = e_6 = \epsilon > 0$.

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In Wu's version of KDP, vertex 1 was not allowed.

We find the partition function Z by the transfer-matrix method originally introduced for the the "ice" problem[6]:

$$Z = \max_y Z(y),$$

where

$$Z(y) = [\Lambda(y)]^N \exp[N^2 E y], \tag{1}$$

and where $E = \mathcal{E}d/kT$ ($\mathcal{E}$ = electric field, d = dipole moment), $y = 1-2n/N$ (n = number of down arrows), and Λ is the maximum eigenvalue of the transfer matrix

$$A(\varphi, \varphi') = \sum \exp(-Km), \tag{2}$$

where $K = \epsilon/kT$ and m = number of types (3)-(6) vertices, and where the sum is over the allowed arrangements of horizontal arrows. The notation in (2) has been fully explained in Refs. 5 and 6. The eigenvalue equation in a given n subspace is [cf. Eq. (1) of Ref. 6]

$$\begin{aligned}\Lambda f(x_1, \cdots, x_n) &= \sum_{y_1=1}^{x_1} \cdots \sum_{y_n=x_{n-1}}^{x_n} f(y_1, \cdots, y_n) D_1(\vec{X}, \vec{Y}) \\ &+ \sum_{y_1=x_1}^{x_2} \cdots \sum_{y_n=x_n}^{N} f(y_1, \cdots, y_n) D_2(\vec{X}, \vec{Y}),\end{aligned} \tag{3}$$

where

$$\begin{aligned}D_1(\vec{X}, \vec{Y}) &= e^{-KN} U(y_2 - x_1) U(y_3 - x_2) \cdots U(y_1 + N - x_n), \\ D_2(\vec{X}, \vec{Y}) &= e^{-KN} U(y_1 - x_1) U(y_1 - x_2) \cdots U(y_n - x_n),\end{aligned} \tag{4}$$

with

$$U(x) e^{K(x-1)} [1 + \delta(x)(e^{2K} - 1)] \tag{5}$$

(δ = Kroenecker delta). It is instructive to compare (4) with the corresponding equation in Ref. 5, whence it will be seen that the KDP model has lost the left/right symmetry inherent in the F model.

Again we make the plane-wave Ansatz

$$f(x_1, \cdots, x_n) = \sum_P a(P) \exp[i \sum_{j=1}^{n} k_{P(j)} x_j], \tag{6}$$

and we find (for n even) the following:

If $P = \cdots p, q, \cdots$ and $Q = \cdots q, p, \cdots$, then $a(P) = a(Q) B(p, q)$ with

$$B(p, q) = -[1 + e^{i(p+q)} - 2\Delta e^{ip}][1 + e^{i(p+q)} - 2\Delta e^{iq}]^{-1},$$

where $\Delta = \frac{1}{2} e^K$.

For all $i = 1, \cdots, n$,

$$\exp(ik_i N) = \prod_{j \neq i} B(k_i, k_j).$$

$$\Lambda = \left\{ \prod_{j=1}^{n} [1 - \exp(ik_j + K)]^{-1} \right\} \left\{ \exp(i \sum_1^n k_j) + e^{-KN} \prod_{j=1}^{n} [\exp(ik_j) - \exp(ik_j + 2K) + e^K] \right\}. \tag{7}$$

Again, we have constructed the eigenvectors of the Heisenberg chain

$$H = -\sum_{i=1}^{N} S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z, \tag{8}$$

although with a different eigenvalue. This time, however, the properties of the ground state of (8) are understood completely only for $\Delta \leq 1$. Nevertheless, we can solve the problem completely for all Δ. It is worth noting that this problem is in some sense the mirror image of the F model.[5] For both models $\Delta = \frac{1}{2}$ corresponds to $T = \infty$. As T decreases, Δ decreases monotonically for the F model with the critical point at $\Delta = -1$. For KDP Δ increases monotonically with $\Delta = +1$ being the critical point. This corresponds to a critical temperature $e^K = 2$. The two models are completely different, however, because the singularities at the two values of Δ are different.

We discuss the high- and low-temperature cases separately:

High temperature ($\frac{1}{2} < \Delta \leq 1$).—Following the standard development,[7] we change variables to $e^{ik} = (e^{i\mu} - e^{\alpha})(e^{i\mu + \alpha} - 1)^{-1}$ with $\Delta = -\cos\mu$.

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The distribution in α space, $R(\alpha)$, satisfies

$$R(\alpha) = \xi(\alpha) - \int_{-b}^{b} K(\alpha-\beta)R(\beta)d\beta, \tag{9}$$

$$\pi(1-y) = \int_{-b}^{b} R(\alpha)d\alpha, \tag{10}$$

with

$$\xi(\alpha) = \sin\mu[\cosh\alpha - \cos\mu]^{-1}, \tag{11}$$

$$K(\alpha) = (2\pi)^{-1}\sin 2\mu[\cosh\alpha - \cos 2\mu]^{-1}. \tag{12}$$

Since the k's are real (with $\sum k = 0$) and since $n < \frac{1}{2}N$ (i.e., $y \geq 0$), the second term in (7) vanishes relative to the first (in the bulk limit). Hence

$$N^{-2}\ln Z(y) = Ey - \frac{1}{4\pi}\int_{-b}^{b} R(\alpha)\ln\left(\frac{\cosh\alpha - \cos 3\mu}{\cosh\alpha - \cos\mu}\right)d\alpha. \tag{13}$$

Since both b and $R(\alpha)$ decrease with increasing y (with $b = \infty$ at $y = 0$) and since the log factor in (13) is negative, it follows that y is an increasing function of E with $y = 0$ at $E = 0$. For $y = 0$, $R(\alpha) = \pi[2\mu\cosh(\pi\alpha/2\mu)^{-1}$ and hence, for $E = 0$,

$$N^{-2}\ln Z = -\frac{1}{4}\int_{-\infty}^{\infty}\frac{d\alpha}{\cosh\pi\alpha}\ln\left(\frac{\cosh 2\mu\alpha - \cos 3\mu}{\cosh 2\mu\alpha - \cos\mu}\right). \tag{14}$$

For $T \sim T_c$, $\mu \approx \pi$ and we can expand the integral in (14) to obtain the internal energy/vertex $= \frac{1}{2}\epsilon$ at $T = T_c$. We also find for $T \sim T_c$ that

$$C \sim (\epsilon^2/4\pi kT^2)(2-e^{K})^{-\frac{1}{2}}. \tag{15}$$

To compute the polarizability for $T \sim T_c$ we expand the logarithm in (13) in powers of $(\cos\mu - \cos 3\mu)(\cosh\alpha - \cos\mu)^{-1}$. The first term so obtained is the same as for the ground-state energy of the Heisenberg chain (8). The dependence of this term on y is known [Ref. 7, Eq. (69)] and we find that

$$N^{-2}\ln[Z(y)/Z(0)] = Ey - \Delta\pi(\pi-\mu)(8\mu)^{-1}(\sin\mu)y^2 + O(y^4) \tag{16}$$

to leading order in $1-\Delta$. This leads to a polarizability

$$\chi \sim 2d^2[k\ln 2(T-T_c)]^{-1}. \tag{17}$$

Low temperature ($\Delta \geq 1$).—We are able to derive the partition function in this case without recourse to (7). Set $E = 0$ and observe that since all energies are non-negative, $Z(y)$ is a convex, continuous, monotonically decreasing function of $\beta = (kT)^{-1}$ (for N finite). Since $z(y) \equiv Z(y)^{1/N^2}$ is bounded above by (4), it follows[8] that as $N \to \infty$, $\lim z$ is a bounded, continuous, convex, nonincreasing function of β. For $N = \infty$ and all y, $z(y) = 1$ at $\beta\epsilon = \ln 2$ [from (13)]. Furthermore, at $\beta = \infty$, $z(y) = 1$ for all y because the completely ordered state has zero energy. [To be precise, if $y = 0$, $Z(0) \geq 2$ (two ordered states). If $y \neq 0$, $Z(y) \geq 2e^{-2\beta\epsilon N}$ which is obtained by placing all the up arrows on a row of vertical bonds next to each other and then placing rows on top of each other in a spiral structure. This introduces two "dislocations" running the length of the lattice. In the bulk limit the factor $\epsilon^{-2\beta\epsilon N}$ is of no consequence.] Now, since z is nonincreasing, we conclude that $z(y) = 1$ for all y and all $T < T_c$. Hence

$$N^{-2}\ln Z(y) = Ey, \text{ or } N^{-2}\ln Z = |E| \quad (\text{for } T < T_c). \tag{18}$$

It is fortunate that we are able to solve the problem this way because it is difficult to obtain the solution from (7). Clearly $\Lambda(0) = 1$ because the product in (7) is vacuous for $n = 0$. When $\Delta > 1$, the appropriate k's are complex and this solution has not yet been found. However, we can evaluate (7) when n is fixed $\gg 1$ and $N \to \infty$. In this case, it is known[9] that $ik_j \equiv p_j$ is real and, as $j \to \infty$, $\cosh p_j$ approaches $\frac{1}{2}\Delta$ rapidly. $N^{-2}\ln\Lambda$ is therefore 0, as required.

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Residual Entropy of Square Ice

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At low temperatures, ice has a residual entropy, presumably caused by an indeterminacy in the positions of the hydrogen atoms. While the oxygen atoms are in a regular lattice, each O–H–O bond permits two possible positions for the hydrogen atom, subject to certain constraints called the "ice condition." The statement of the problem in two dimensions is to find the number of ways of drawing arrows on the bonds of a square planar net so that precisely two arrows point into each vertex. If N is the number of molecules and (for large N) W^N is the number of arrangements, then $S=Nk\ln W$. Our exact result is $W=(\frac{4}{3})^{3/2}$.

I. INTRODUCTION

MANY simple substances are observed to have a *residual entropy*, which is to say that at temperatures well below the freezing point there is a *constant* entropy much larger than that caused by any conceivable lattice vibrations. "For example, the observed entropy of crystalline hydrogen shows that even at very low temperature the molecules of orthohydrogen in the crystal are rotating about as freely as in the gas."[1] Most substances with this property are, like water, hydrogen-bonded, although there are notable exceptions such as carbon monoxide and nitrous oxide.

Thirty-four years ago, it was realized that ice also falls in this category when Giauque and Ashley[2] calculated the entropy of gaseous water from its band spectrum and compared the result with $\int C_p d\ln T$ from previous specific-heat data. Three years later, Giauque and Stout[3] accurately remeasured the specific heat of water from 15 to 273°K, being very careful to cool the water slowly to ensure thermal equilibrium. They obtained an entropy of 44.28±0.05 cal/deg mole for gaseous water at 1 atm and 298.1°K, which was less than the spectroscopic value by 0.82±0.05 cal/deg mole. (In arriving at this result, the specific heat between 10 and 15°K was extrapolated from their data and agreed closely with previous measurements of Simon[3] between 9 and 13°K; the entropy at 10°K was calculated from a Debye model and amounted to only 0.022 cal/deg mole, which is a small fraction of the total discrepancy.) They also mention that "MacDougall and Giauque[4] investigated ice from 0.2 to 4°K and found no appreciable heat capacity in this range."

The structure of ice, as determined from x-ray data, is one in which the oxygen atoms are regularly arranged in a crystal lattice. Technically, it is a hexagonal wurtzite structure,[5] but it is simpler to think of it as a distorted tetrahedral diamond structure—for the important point is that each oxygen atom has four nearest neighbors. The hydrogen atoms, however, do not appear to have any regular arrangement discernible by x-rays.

Amplifying earlier ideas of Bernal and Fowler,[6] Pauling[1] made the following hypotheses:

(a) Ice is hydrogen-bonded with one hydrogen atom between every pair of nearest-neighbor oxygen atoms. Since the observed O-O distance is 2.76 Å and since the O-H bond is well known to be only 0.95 Å in the gas, there are two possible positions for each hydrogen atom, these being approximately 0.95 Å from each end of the O-O line. These states are energetically equivalent except for

(b) *The ice condition:* "The concentration of $(OH)^-$ and $(H_3O)^+$ ions in water is very small and we expect the situation to be essentially unchanged in ice."[1] Consequently, each oxygen atom must be surrounded by two hydrogen atoms near to it (0.95 Å) and two on the far side (1.81 Å).

This ice condition can be pictured geometrically by constructing a lattice of coordination number four and by drawing arrows on and parallel to each bond in such a manner that there are precisely two arrows pointing into each vertex. The entropy is then

$$S=Nk\ln W, \tag{1.1}$$

where N is the number of oxygens (vertices), k is Boltzmann's constant, and $Z\equiv W^N$ and is equal to the number of ways of arranging the arrows (for N large). If we ignore the ice condition, then $Z\equiv W^N=2^{2N}$ (because there are $2N$ bonds) and $W=4$. This leads to an entropy that is much too large.

Pauling[1] made a rough estimate of W in the following way: Suppose that the bonds and the vertex configurations are independent (they are not). Then

$$Z\cong 2^{2N}(6/16)^N \quad \text{or} \quad W\cong 1.5, \tag{1.2}$$

where the factor 6/16 comes from the fact that we permit only six out of a total of 16 *a priori* vertex

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configurations. This estimate leads to an entropy of 0.805 cal/deg mole, which is in excellent agreement with the observed value and which must be counted as one of the most successful applications of elementary statistical mechanics to real substances.

Plainly, it is important to improve the calculation of W because W is a sensitive indicator of the soundness of the hypothesized structure of ice. The best numerical estimate of W is due to Nagle,[5,7] who found

$$W_{\text{real ice}}=1.50685\pm0.00015\,, \tag{1.3}$$

or $S=0.8145\pm0.0002$ cal/deg mole. It is truly remarkable that the accurate value (1.3) is so close to the crude estimate (1.2).

It is also possible to consider "square ice," which is the subject matter of this paper. Square ice is the two-dimensional version of real ice and is defined by the same ice condition applied to a square planar lattice (as in the usual Ising model). Nagle gives

$$W_{\text{square ice}}=1.540\pm0.001\,. \tag{1.4}$$

It seemed worthwhile to try to find the value of $W_{\text{square ice}}$ exactly for the following reasons: (a) It will serve as a check on the accuracy of Nagle's calculations. (b) It is an interesting graph theoretic problem. (c) It is the first step toward the solution of much more interesting models having phase transitions—the Rys antiferromagnetic F model and the Slater KDP model of a ferroelectric.[8] (It is believed that hydrogen-bonded ferro and antiferroelectrics have the same "rules" as ice except that the six vertex configurations have different energies according to the total polarization at each vertex. See the Appendix.)

Here we calculate $W_{\text{square ice}}$ exactly by the method of the transfer matrix and our result[9] is

$$W_{\text{sq. ice}}=(\tfrac{4}{3})^{3/2}=1.5396007\cdots\,. \tag{1.5}$$

II. THE TRANSFER MATRIX

Let the square lattice consist of NM vertices (N horizontally and M vertically). The number of bonds is thus $2NM$, half of which are vertical and half horizontal; these bonds will be called V bonds and H bonds, respectively. Beginning at the bottom, we have a row of NV bonds followed by a row of H bonds and so on alternately. There are M bond rows of each type.

Let φ denote a possible configuration of a row of V bonds, i.e., a definite assignment of up or down arrows on each of the NV bonds. There are obviously 2^N choices for φ. Alternatively, φ may be thought of as a state of a linear chain of N spin-$\frac{1}{2}$ particles (in the S^z representation). If φ and φ' are the configurations of two successive rows of V bonds, let $A(\varphi,\varphi')$ be the number of ways of assigning arrows on the intervening row of H bonds so that the ice condition is satisfied at each of the N vertices lying on the intervening row. Thus $A(\varphi,\varphi')$ is a non-negative integer. If Z is the total number of ways of correctly placing arrows on the lattice, we have

$$Z=\sum_{\varphi_1}\cdots\sum_{\varphi_M}A(\varphi_1,\varphi_2)A(\varphi_2,\varphi_3)\cdots A(\varphi_{M-1},\varphi_M)A(\varphi_M,\varphi_1)$$
$$=[\mathrm{Tr}A]^M. \tag{2.1}$$

In (2.1), $\sum_{\varphi_j}$ means a sum on the 2^N states of the jth row of V bonds. Implicit in (2.1) is the fact that the Mth row is connected by V bonds to the first row. As usual (for large M),

$$Z=\Lambda^M\,, \tag{2.2}$$

where Λ is the largest eigenvalue of the 2^N-square matrix A. The quantity W is thus given by

$$\ln W=\lim_{N\to\infty}N^{-1}\ln\Lambda\,. \tag{2.3}$$

Next, we must elucidate the elements of A. If $\varphi=\varphi'$, there are two possible assignments of horizontal arrows, all running to the left or all running to the right. Thus,

$$A(\varphi,\varphi)=2\,. \tag{2.4}$$

To simplify the subsequent discussion let us also assume that the lattice is wrapped on a torus instead of merely on a cylinder, i.e., that the Nth column is connected by H bonds to the first column. If $\varphi\neq\varphi'$, then certain up arrows in φ are replaced by down arrows in φ' (a $+-$ exchange) and vice versa (a $-+$ exchange). In order to satisfy the ice condition, the intervening horizontal arrows must point outwards on both sides of a $+-$ vertex and inwards at a $-+$ vertex If there is no change at a vertex, the two horizontal arrows can be either both to the right or both to the left. Thus,

$$A(\varphi,\varphi')=1 \tag{2.5}$$

if and only if there is a $-+$ exchange between every pair of $+-$ exchanges and vice versa, and if there is an equal number of both kinds of exchange. Otherwise

$$A(\varphi,\varphi')=0\,. \tag{2.6}$$

To interpret the above rule in spin language, A is

[7] Earlier estimates were made by E. A. DiMarzio and F. H. Stillinger, J. Chem. Phys. **40**, 1577 (1964); H. Takahasi, Proc. Phys. Math. Soc. (Japan) **23**, 1069 (1941).

[8] F. Rys, Helv. Phys. Acta **36**, 537 (1963); J. C. Slater, J. Chem. Phys. **9**, 16 (1941); see also J. F. Nagle [J. Math. Phys. **7**, 1492 (1966)] for useful pictures and a bibliography of earlier work. The solution to the F model is reported in E. H. Lieb, Phys. Rev. Letters **18**, 1046 (1967) and the KDP model **19**, 108 (1967).

[9] A summary of this work was given in E. H. Lieb, Phys. Rev. Letters **18**, 692 (1967).

obviously the same as

$$\mathfrak{A}=2+\sum_{i<j} S_i^- S_j^+ + \sum_{i<j<k<l} S_i^- S_j^+ S_k^- S_l^+ + \cdots + (S_1^- S_2^+ \cdots S_N^+) + \sum_{i<j} S_i^+ S_j^- + \sum_{i<j<k<l} S_i^+ S_j^- S_k^+ S_l^- + \cdots + (S_1^+ S_2^- \cdots S_N^-), \quad (2.7)$$

where we have assumed that N is even in the last term.

From (2.7) we see that $S^z=\sum_1^N S_i^z$ is a constant of the motion, i.e., if n is the number of down arrows in a state φ, then $A(\varphi,\varphi')=0$ unless $n=n'$. $S^z=\frac{1}{2}N-n$. Since A is thus a diagonal block matrix we must decide in which n subspace the maximum eigenvalue lies. Intuition dictates that it is the subspace $n=\frac{1}{2}N$ or $\frac{1}{2}(N-1)$ (i.e., $S^z=0$ or $\frac{1}{2}$) if N is even or odd, respectively. While we can not prove this statement for finite N, we can prove a statement that is sufficient for our purposes, namely, that as $N\to\infty$,

$$N^{-1}\ln\Lambda_{\max}(\text{all } n)=N^{-1}\ln\Lambda_{\max}(n=\tfrac{1}{2}N).$$

This weaker assertion is proved in a general way in the Appendix. It will also be proved in a specific way in Sec. IV when we actually display the largest eigenvalue as a function of n/N in the limit $N\to\infty$.

Since A is non-negative, and since any φ can be connected to every other φ' in the same n subspace by applying A a sufficient number of times, it follows, by the Perron-Fröbenius theorem, that the largest eigenvector in each subspace is nondegenerate and has strictly positive components. This observation will prove to be extremely useful because it will enable us to identify the largest eigenvectors.

It is very fortunate that the largest eigenvalue can be sought in the $n=\frac{1}{2}N$ subspace, for only in this subspace can the calculation be carried to completion. In all other subspaces, the largest eigenvalue must be left as the solution to a linear, but unsolvable, integral equation [cf. (4.8′)].

To proceed, we must find a more tractable form for A than (2.7). Denote by $\varphi(x_1,\ldots,x_n)$ the state (in a given n space) with down arrows (spins) at the sites $1\le x_1<x_2<\cdots<x_n\le N$. Any eigenvector Ψ, of A, may be written as

$$\Psi=\sum_{x_1,\cdots,x_n} f(x_1,\ldots,x_n)\varphi(x_1,\ldots,x_n) \quad (2.8)$$

and the equation $A\Psi=\Lambda\Psi$ implies some corresponding equation for the set of $\binom{N}{n}$ coefficients f. We shall write it down and justify it afterwards:

$$\Lambda f(x_1,\ldots x_n)=\sum_{y_1=1}^{x_1}\sum_{y_2=x_1}^{x_2}\cdots\sum_{y_n=x_{n-1}}^{x_n} f(y_1,\ldots,y_n) + \sum_{y_1=x_1}^{x_2}\sum_{y_2=x_2}^{x_3}\cdots\sum_{y_n=x_n}^{N} f(y_1,\ldots,y_n). \quad (2.9)$$

Equation (2.9) is true only in the region R,

$$R:\ 1\le x_1<x_2<\cdots<x_n\le N, \quad (2.10)$$

which is the region in which f is defined. On the right side of (2.9), therefore, f must be taken to be zero if any $y_j=y_{j+1}$ (e.g., $y_1=y_2=x_1$).

To verify (2.9) we ask what states $\varphi(x_1,\ldots,x_n)$ are generated when A acts on a state $\varphi(y_1,\ldots,y_n)$ according to the rules stated above. If $y_j=x_j$ (all j) then $A=2$, and this is in accord with (2.9). [We get one from the upper limits of the first sum and one from the lower limits of the second sum in (2.9).] If $\mathbf{Y}\neq\mathbf{X}$ there are two possibilities: (a) the first exchange reading from the left to the right (i.e., from 1 to N) is a $-+$ exchange, the second is a $+-$ exchange, and so on; (b) the reverse of (a). In order to produce a given state $\varphi(x_1,\ldots,x_n)$ by possibility (a), it is clearly necessary and sufficient that the y_i satisfy

$$x_1\le y_1\le x_2,\ x_2\le y_2\le x_3,\ldots,\ x_n\le y_n\le N, \quad (2.11)$$

but not $y_i=x_i$ (*all* i). If (2.11) is satisfied, then application of A to $\varphi(\mathbf{Y})$ produces $\varphi(\mathbf{X})$ with coefficient unity, (2.5). All these matrix elements are contained the correct number of times in the second sum of (2.9). *Mutatis mutandis*, possibility (b) is contained in the first sum of (2.9).

III. DIAGONALIZATION OF THE TRANSFER MATRIX

We now make an ansatz for f and will verify that it leads to the maximum eigenvalue. Let

$$f(y_1,\ldots,y_n)=\sum_P ! a(P)\exp\left[i\sum_{j=1}^{n} k_{P(j)}y_j\right]. \quad (3.1)$$

In (3.1) $\{k\}=k_1, k_2,\ldots, k_n$ is a set of N wave numbers and the sum is on $n!$ permutations with certain coefficients $a(P)$. The goal is to choose $a(P)$ and $\{k\}$ so that (2.9) is satisfied. We will also assume that $k_i\neq 0$ (all i) and it will turn out that this assumption is justified if n is even. [We shall not consider the case of n odd. For that case the assumption (3.1) is probably also correct (we have verified it for $n=3$) but the subsequent analysis has to be somewhat modified.]

When (3.1) is inserted into the right side of (2.9) we must remember to sum only over configurations $\mathbf{Y}=(y_1,\ldots,y_n)$ that are in R, (2.10). To do this we will sum (3.1) over all $\mathbf{Y}$ and then explicitly subtract those terms in (2.9) for which one or more $y_i=y_{i+1}$. We shall call these subtracted terms diagonal terms. To clarify this point, suppose $n=2$ and suppose, for simplicity, that $f(y_1,y_2)=\exp(iky_1+iqy_2)$, i.e., a single plane wave. Then, the first sum in (2.9) would give

$$\sum_{y_1=1}^{x_1}\sum_{y_2=x_1}^{x_2} f(y_1,y_2)-f(x_1,x_1) = \alpha(k)\alpha(q)\{e^{ik}-e^{ik(x_1+1)}\}\{e^{iqx_1}-e^{iq(x_1+1)}\}-e^{i(k+q)x_1},$$

where

$$\alpha(k)=[1-e^{ik}]^{-1}. \tag{3.2}$$

Likewise, the second sum in (2.9) would give

$$\alpha(k)\alpha(q)\{e^{ikx_1}-e^{ik(x_2+1)}\}\{e^{iqx_2}-e^{iq(N+1)}\}-e^{i(k+q)x_2}.$$

Thus, for general n (even), performing the first sum or some single plane wave, $\exp i(k_1y_1+\cdots+k_ny_n)$, gives

$$\prod_{j=1}^{n}\alpha(k_j)\{e^{ik_1}-e^{ik_1(x_1+1)}\}\{e^{ik_2x_1}-e^{ik_2(x_2+1)}\}\cdots$$

$$\{e^{ik_nx_{n-1}}-e^{ik_n(x_n+1)}\}-(\text{diagonal terms}), \tag{3.3}$$

while the second sum gives

$$\prod_{j=1}^{n}\alpha(k_j)\{e^{ik_1x_1}-e^{ik_1(x_2+1)}\}\{e^{ik_2x_2}-e^{ik_2(x_3+1)}\}\cdots$$

$$\{e^{ik_nx_n}-e^{ik_n(N+1)}\}-(\text{diagonal terms}). \tag{3.4}$$

If we study (3.3) we see that it contains precisely one term that is proportional to one of the plane waves in (3.1) and that plane wave is, in fact, the very one we started with, namely, the term

$$\left\{\prod_{j=1}^{n}\alpha(k_j)\right\}\exp\left[i\sum_{1}^{n}k_j\right]\exp\left[i\sum_{1}^{n}k_jx_j\right]. \tag{3.5}$$

(Remember that n is even so that there are an even number of minus signs.) All the other terms—the diagonal terms as well as those coming from the curly brackets—have the property that one or more of the x_i's fail to appear. These other terms are unwanted and must be made to cancel.

Likewise, the second sum, (3.4), gives a single wanted term

$$\left\{\prod_{j=1}^{n}\alpha(k_j)\right\}\exp\left[i\sum_{1}^{n}k_jx_j\right], \tag{3.6}$$

the remaining terms being unwanted.

In both (3.5) and (3.6) the coefficient of the wanted term is invariant with respect to any permutation of the set $\{k\}$. Therefore, assuming that we can choose the coefficients $a(P)$ and the set $\{k\}$ so as to eliminate the unwanted terms, (2.9) will be satisfied with an eigenvalue

$$\Lambda=\left\{\prod_{j=1}^{n}\alpha(k_j)\right\}\left\{1+\exp\left[i\sum_{1}^{n}k_j\right]\right\}. \tag{3.7}$$

It is indeed possible to eliminate the unwanted terms. We shall state the requirements and then verify by induction that they suffice:

(1) Condition on $a(P)$: Let P and Q be two permutations of $\{k\}$ that are identical except for the jth and $(j+1)$th position, i.e., $P\{k\}=(\cdots p,q\cdots)$ and $Q\{k\}=(\cdots q,p\cdots)$. Then,

$$a(P)=a(Q)B(p,q), \tag{3.8}$$

with

$$B(p,q)=-\frac{1+e^{i(p+q)}-e^{ip}}{1+e^{i(p+q)}-e^{iq}},$$

$$=-\exp[-i\Theta(p,q)], \tag{3.9}$$

where

$$\tan\tfrac{1}{2}\Theta(p,q)=\frac{\sin\tfrac{1}{2}(p-q)}{2\cos\tfrac{1}{2}(p+q)-\cos\tfrac{1}{2}(p-q)}. \tag{3.10}$$

We assume p and q are real and Θ is continuous with $\Theta(0,0)=0$. The solution to (3.8) is unique, except for a normalization constant, and is

$$a(P)=(-)^P\exp\left[-\frac{i}{2}\sum_{i<j}\Theta(k_{P(i)}k_{P(j)})\right]. \tag{3.11}$$

(2) Condition on $\{k\}$: For each $j=1,\cdots,n$

$$\exp(ik_jN)=-\prod_{i\neq j}B(k_j,k_i). \tag{3.12}$$

An alternative, equivalent statement of (3.12), using (3.8), is this: For every pair of cyclically related permutations,

$$P=[P(1),P(2),\cdots,P(n)]$$

and

$$Q=[P(2),P(3),\cdots,P(n),P(1)],$$

we have

$$a(P)=[\exp ik_{P(1)}N]a(Q). \tag{3.13}$$

We now give an inductive proof that (3.8) and (3.13) guarantee that the ansatz (3.1) satisfies (2.9) with eigenvalue (3.7). A simple artifice to insure that we sum only over R is to introduce the factor

$$w^n(y_1,\ldots,y_n)=\prod_{j=1}^{n-1}[1-\delta(y_{j+1}-y_j)] \tag{3.14}$$

into the sums in (2.9). Here, δ is the Kroenecker delta [$\delta(x)=1$ if $x=0$; $\delta(x)=0$, otherwise]. However, since $x_{j+1}>x_j$ (all j), we can make the following replacement in the first sum, S_1:

$$S_1\colon\ \delta(y_{j+1}-y_j)=\delta(y_{j+1}-x_j)\delta(y_j-x_j). \tag{3.15a}$$

Likewise, in the second sum, S_2:

$$S_2\colon\ \delta(y_{j+1}-y_j)=\delta(y_{j+1}-x_{j+1})\delta(y_j-x_{j+1}). \tag{3.15b}$$

Now, multiply (3.1) by $w^n(y_1,\ldots,y_n)$, insert the product into the first sum in (2.9), and perform the

indicated sums on $y_n, y_{n-1}, \cdots, y_{n-t+1}$ *only*. The partial sum thus obtained is clearly of the form

$$S_1^t = w^{n-t}(y_1,\cdots,y_{n-t}) \sum_P {}' \left\{ a(P) \exp\left[i \sum_{j=1}^{n-t} k_{P(j)} y_j \right] \times G_P^t(x_{n-t}, x_{n-t+1},\cdots,x_n;\, y_{n-t}) \right\} . \quad (3.16)$$

Our inductive premise for G_P^t is the following (for $1 \le t \le n-1$):

$$G_P^t(x_{n-t},\cdots,x_n;\, y_{n-t}) = \prod_{j=n-t+1}^{n} \{-\alpha(k_{P(j)}) \exp[ik_{P(j)}(x_j+1)]\} + [\exp(ik_{P(n-t+1)}x_{n-t})\{\alpha(k_{P(n-t+1)}) - \delta(y_{n-t}-x_{n-t})\} \times g_P^t(x_{n-t+1},\cdots,x_n)], \quad (3.17)$$

where g_P^t *does not depend upon* $P(1), P(2), \cdots, P(n-t+1)$.

To prove (3.17) for $t=1$, we must do the sum on y_n. Suppressing irrelevant factors, this means that for each P we must do the sum

$$\sum_{y_n=x_{n-1}}^{x_n} [1-\delta(y_n-x_{n-1})\delta(y_{n-1}-x_{n-1})] \exp[ik_{P(n)}y_n] = \alpha(k_{P(n)})\{\exp[ik_{P(n)}x_{n-1}] - \exp[ik_{P(n)}(x_n+1)]\} - \delta(y_{n-1}-x_{n-1}) \exp[ik_{P(n)}x_{n-1}]. \quad (3.18)$$

Clearly, (3.18) is of the form (3.16) and (3.17), with

$$g_P^1(x_n) = 1. \quad (3.19)$$

To carry through the induction, we must sum (3.16) on y_{n-t}. Again, suppressing irrelevant factors, we must do the sum

$$\sum_{y_{n-t}=x_{n-t-1}}^{x_{n-t}} [1-\delta(y_{n-t}-x_{n-t-1})\delta(y_{n-t-1}-x_{n-t-1})] \times \exp[ik_{P(n-t)}y_{n-t}] G_P^t(x_{n-t},\cdots,x_n;\, y_{n-t}). \quad (3.20)$$

The first term on the right side of (3.17), when inserted into (3.20), gives

$$\prod_{j=n-t}^{n} \{-\alpha(k_{P(j)}) \exp[ik_{P(j)}(x_j+1)]\} + \left\{ \prod_{j=n-t+1}^{n} [-\alpha(k_{P(j)}) \exp[ik_{P(j)}(x_j+1)]] \right\} \times \exp[ik_{P(n-t)}x_{n-t-1}] \times \{\alpha(k_{P(n-t)}) - \delta(y_{n-t-1}-x_{n-t-1})\}. \quad (3.21)$$

The second term of (3.17) gives

$$g_P^t(x_{n-t+1},\cdots,x_n) \exp[ik_{P(n-t+1)}x_{n-t}] \times \{\alpha(k_{P(n-t+1)})[\alpha(k_{P(n-t)}) \times \{\exp[ik_{P(n-t)}x_{n-t-1}] - \exp[ik_{P(n-t)})(x_{n-t}+1)]\} - \delta(y_{n-t-1}-x_{n-t-1}) \exp[ik_{P(n-t)}x_{n-t-1}]] - \exp[ik_{P(n-t)}x_{n-t}]\}. \quad (3.22)$$

[It is important to recall that $\delta(y_{n-t}-x_{n-t}) \times \delta(y_{n-t}-x_{n-t-1}) = 0$.]

When we multiply out the exponential factors in (3.22) we observe that there are some terms in which x_{n-t} occurs twice, namely,

$$-\{\alpha(k_{P(n-t+1)})\alpha(k_{P(n-t)}) \times \exp[ik_{P(n-t)}]+1\} g_P^t(x_{n-t+1},\cdots,x_n) \times \exp[i(k_{P(n-t)}+k_{P(n-t+1)})x_{n-t}]. \quad (3.23)$$

We would like to make (3.23) vanish. That it does so is a consequence of (3.8), for observe that (a) g_P^t is independent of $P(n-t+1)$ and $P(n-t)$; (b) for each permutation $P = \cdots P(n-t), P(n-t+1), \cdots$ in (3.16) that gives rise to a term (3.23) there is a permutation $Q = \cdots P(n-t+1), P(n-t)\cdots$ that gives rise to a term with the same exponential dependence on x_{n-t}, but with a different coefficient. Each such pair of terms will vanish if

$$a(P)\{\alpha(k_{P(n-t+1)})\alpha(k_{P(n-t)}) \exp[ik_{P(n-t)}]+1\} + a(Q)\{\alpha(k_{P(n-t)})\alpha(k_{P(n-t+1)}) \times \exp[ik_{P(n-t+1)}]+1\} = 0. \quad (3.24)$$

Using (3.2), condition (3.24) is seen to be identical to (3.8). Consequently, (3.23) can be omitted from (3.22).

Combining the remainder of (3.22) with (3.21), we verify (3.17) for $t+1$ with

$$g_P^{t+1}(x_{n-t},\cdots,x_n) = \prod_{j=n-t+1}^{n} \{-\alpha(k_{P(j)}) \exp[ik_{P(j)}(x_j+1)]\} + g_P^t(x_{n-t+1},\cdots,x_n)\alpha(k_{P(n-t+1)}) \times \exp[ik_{P(n-t+1)}x_{n-t}]. \quad (3.25)$$

Equation (3.25) also verifies that g_P^{t+1} is independent of $P(n-t)$.

The induction proceeds up to and including $t=n-1$. The final summation on y_1 is slightly different, because there is neither a y_0 nor an x_0, but the same reasoning as above gives

$$G_P^n(x_1,\cdots,x_n) = \prod_{j=1}^{n} \{-\alpha(k_{P(j)}) \exp[ik_{P(j)}(x_j+1)]\} + \exp[ik_{P(1)}]\alpha(k_{P(1)})g_P^n(x_1,\cdots,x_n), \quad (3.26)$$

with g_P^n being given correctly by (3.25) with $t=n-1$.

The obvious significance of $G_P{}^n$ is that

$$S_1=\sum_P{}' a(P)G_P{}^n(x_1,\cdots,x_n). \tag{3.27}$$

We turn now to the second sum S_2, of (3.29). This we will do in reverse order, namely, $y_1,y_2,\cdots,y_t$. The partial sum will be denoted $S_2{}^t$. The procedure is exactly the same, *mutatis mutandis*, as for S_1, and it suffices merely to quote the final result, i.e., the analogs of (3.16), (3.17), (3.19), (3.25), (3.26), and (3.27). The analogs of G and g will be denoted by H and h, respectively.

$$S_2=w^{n-t}(y_{t+1},\cdots,y_n)\times\sum_P{}'\left\{a(P)\exp\left[i\sum_{j=t+1}^{n}k_{P(j)}y_j\right]\times H_P{}^t(x_1,\cdots,x_{t+1};\,y_{t+1})\right\}. \tag{3.28}$$

$$H_P{}^t(x_1,\cdots,x_{t+1};\,y_{t+1})=\prod_{j=1}^{t}\{\alpha(k_{P(j)})\exp[ik_{P(j)}x_j]\}+(-1)^t[\exp[ik_{P(t)}(x_{t+1})]\times\{\alpha(k_{P(t)})\exp[ik_{P(t)}]+\delta(y_{t+1}-x_{t+1})\}\times h_P{}^t(x_1,\cdots,x_t)]. \tag{3.29}$$

$$h_P{}^1(x_1)=1. \tag{3.30}$$

$$h_P{}^{t+1}(x_1,\cdots,x_{t+1})=\prod_{j=1}^{t}\{-\alpha(k_{P(j)})\exp[ik_{P(j)}x_j]\}+h_P{}^t(x_1,\cdots,x_t)\alpha(k_{P(t)})\times\exp[ik_{P(t)}(x_{t+1}+1)]. \tag{3.31}$$

$$H_P{}^n(x_1,\cdots,x_n)=\prod_{j=1}^{n}\{\alpha(k_{P(j)})\exp[ik_{P(j)}x_j]\}+\exp[ik_{P(n)}(N+1)]\alpha(k_{P(n)})\times h_P{}^n(x_1,\cdots,x_n), \tag{3.32}$$

with $h_P{}^n$ being given by (3.31) with $t=n-1$. Again,

$$S_2=\sum_P{}' a(P)H_P{}^n(x_1,\cdots,x_n). \tag{3.33}$$

When we compute S_1 and S_2 with (3.27) and (3.33) we note that the first terms in (3.26) and (3.32) give us exactly what we want, namely, $\Delta f(x_1,\cdots,x_n)$. The second terms in (3.27) and (3.33) must be made to cancel, and to do this we must investigate $g_P{}^n$ and $h_P{}^n$ more closely.

From the initial statement (3.19) and the recursion relation (3.25), it is easy to deduce that $g_P{}^t$ consists of t terms which, for $t>1$, are given by

$$g_P{}^t(x_{n-t+1},\cdots,x_n)=\left\{\prod_{j=n-t+2}^{n}[\alpha(k_{P(j)})]\right\}\sum_{s=1}^{t}(-1)^{s+t}\times\exp\left[i\sum_{j=n-t+2}^{n}k_{P(j)}M_j{}^s\right], \tag{3.34}$$

where, for $1<s<t$,

$$\begin{aligned}M_j{}^s&=x_{j-1}, &&\text{for } n-t+2\le j\le n-t+s\\&=x_j+1, &&\text{for } n-t+s+1\le j\le n,\end{aligned} \tag{3.35}$$

while for $s=1$,

$$M_j{}^1=x_j+1, \tag{3.36}$$

and for $s=t$,

$$M_j{}^t=x_{j-1}. \tag{3.37}$$

Conversely, using the recursion relation (3.31) and the initial relation (3.30) for $h_p{}^t$ we find, for $t>1$,

$$h_P{}^t(x_1,\cdots,x_t)=\left\{\prod_{j=1}^{t-1}[\alpha(k_{P(j)})]\right\}\sum_{s=1}^{t}(-1)^{s+t}\times\exp\left[i\sum_{j=1}^{t-1}k_{P(j)}N_j{}^s\right], \tag{3.38}$$

where, for $1<s<t$,

$$\begin{aligned}N_j{}^s&=x_j, &&\text{for } 1\le j\le t-s\\&=x_{j+1}+1, &&\text{for } t-s+1\le j\le t-1,\end{aligned} \tag{3.39}$$

while for $s=1$,

$$N_j{}^1=x_j \tag{3.40}$$

and for $s=t$,

$$N_j{}^t=x_{j+1}+1. \tag{3.41}$$

When $t=n$, comparison of (3.38) and (3.34) shows that $g_P{}^n$ and $h_P{}^n$ are very similar. The relationship is simply this: Let P and Q be two cyclically related permutations, i.e., $P=[P(1),P(2),\cdots,P(n)]$ and $Q=[P(2),P(3),\cdots,P(n),P(1)]$. Then

$$-h_Q{}^n(x_1,\cdots,x_n)=g_P{}^n(x_1,\cdots,x_n). \tag{3.42}$$

Consider now the unwanted terms in S_1+S_2, i.e., the second terms on the right-hand sides of (3.32) and (3.26). These are

$$\sum_P{}' a(P)\{\exp[ik_{P(n)}(N+1)]\alpha(k_{P(n)})h_P{}^n(x_1,\cdots,x_n)+\exp[ik_{P(1)}]\alpha(k_{P(1)})g_P{}^n(x_1,\cdots,x_n)\}. \tag{3.43}$$

Since the sum in (3.43) is over all permutations we see, using (3.42), that (3.43) vanishes identically if

$$a(P)=a(Q)\exp[ik_{P(1)}N] \tag{3.44}$$

for every pair of cyclically related permutations as above. But (3.44) is the same as our second condition, (3.13).

To summarize the results of this section, for every set of numbers $\{k\}$ satisfying (3.13) and such that no $k_j=0$, we have a solution to the eigenvalue problem with an eigenvalue given by (3.7). The existence and determination of such a solution and the proof that it is, in fact, the largest eigenvalue is the subject of Sec. IV.

IV. DETERMINATION OF THE LARGEST EIGENVALUE

We are indeed very fortunate that Eqs. (3.13) and (3.8) have appeared previously in the literature in another context and have been discussed extensively. Consider the linear chain anisotropic Heisenberg ferromagnet with the Hamiltonian

$$H'=-2\sum_{j=1}^{N} S_j^x S_{j+1}^x+S_j^y S_{j+1}^y+\Delta S_j^z S_{j+1}^z, \quad (4.1)$$

with $S_{N+1}=S_1$. To find the eigenvectors of (4.1), in a given S^z (or n) subspace one makes exactly the same ansatz (3.1) as we have done (known as the Bethe hypothesis). In the particular case $\Delta=\frac{1}{2}$, the resulting equations are exactly the same as our (3.8)–(3.13). Yet, while the eigenvectors of (4.1) and (3.7) are the same, the eigenvalues are quite different. For H' the eigenvalue is

$$E=-(\Delta/2)N+2\sum_{j=1}^{n}(\Delta-\cos k_j). \quad (4.2)$$

The fact that the eigenvalues (4.2) and (3.7) are different is immaterial to the discussion of the existence and value of the set $\{k\}$.

The most recent and complete discussion of (4.1) is due to Yang and Yang.[10] In their first paper, YY prove that the ansatz (3.1) in fact gives the ground state of (4.1) in all n subspaces with $n\leq N/2 (S^z\geq 0)$. The set $\{k\}$ which gives this ground state [and thereby satisfies (3.13)] is real and has the property (YY I.9)

$$-(\pi-\mu)<k_j<\pi-\mu, \quad (\text{all } j) \quad (4.3)$$

with (YY I.10)

$$\cos\mu=-\Delta. \quad (4.4)$$

In our case $\Delta=\frac{1}{2}$, so that

$$\mu=\tfrac{2}{3}\pi. \quad (4.5)$$

We also note that the ground-state eigenfunction of (4.1), when written in the S_z representation (2.8), has the property that the f coefficients are strictly positive (for the same reason that they are positive in our problem). In both cases, these positive eigenfunctions are unique in the sense that there can be only one eigenfunction with this positivity property for each problem.

Another property of $\{k\}$ (YY I.35 and theorem 1) is this:

$$k_i\neq k_j \quad (\text{for } i\neq j) \quad (4.6)$$

and the k's may be ordered so that

$$k_j=-k_{n-j+1}. \quad (4.7)$$

Hence, for n even, $k_j\neq 0$ (all j) and our previous analysis in Sec. III is justified.

These observations together with the YY proof mentioned above establish that there is a solution $\{k\}$ to our Eqs. (3.8) and (3.13) and that this solution leads to an eigenfunction which is simultaneously the ground state of (4.1) and the maximum eigenvector of our transfer matrix.

In their second paper, YY evaluate the set $\{k\}$ as $N\to\infty$. One assumes that as n, $N\to\infty$ with n/N = fixed const., the k's fill some interval $-Q\leq k\leq Q$ (with $Q\leq\pi-\mu$) and that the k's fill this interval without any gaps with a density function $\rho(k)$. That is, the number of k's between k and $k+dk$ approaches $N\rho(k)dk$. While all previous workers have made this assumption, it has to be admitted that a rigorous proof is lacking. YY promise a rigorous proof in a later paper, however (YY II.2 *et seq.*).

Given the assumption of a density function, (3.12) leads to the following integral equation (YY II.6a):

$$1=2\pi\rho(k)-\int_{-Q}^{Q}\frac{\partial\theta(k,q)}{\partial k}\rho(q)dq, \quad (4.8)$$

while the equation that determines Q is (YY II.6b)

$$\frac{n}{N}=\int_{-Q}^{Q}\rho(q)dq. \quad (4.9)$$

YY II prove that (4.8) and (4.9) have a unique solution which is positive (as it should be) and that Q is a differentiable, increasing function of n/N with $Q=\pi-\mu$ for $n/N=\frac{1}{2}$.

To solve (4.8) it is convenient to make a change of variables (YY I.21g and 21h) from k to α:

$$e^{ik}=(e^{i\mu}-e^{\alpha})(e^{i\mu+\alpha}-1)^{-1}. \quad (4.10)$$

If we define a density R for α, so that $R(\alpha)d\alpha=2\pi\rho(k)dk$, then (4.8) and (4.9) become (YY II.7a, 7b and Table II)

$$R(\alpha)=\xi(\alpha)-(2\pi)^{-1}\int_{-b}^{b}K(\alpha-\beta)R(\beta)d\beta, \quad (4.8')$$

[10] C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966); **150**, 327 (1966). References to equations in these two papers will be denoted (YYI.21) and (YYII.21), respectively. The reader is also referred to these papers for a bibliography of previous work. See also J. des Cloizeaux and M. Gaudin, J. Math. Phys. **7**, 1384 (1966).

$$2\pi\frac{n}{N}=\int_{-b}^{b}R(\alpha)d\alpha, \tag{4.9'}$$

where

$$\xi(\alpha)=\sin\mu[\cosh\alpha-\cos\mu]^{-1}, \tag{4.11}$$

$$2\pi K(\alpha)=\sin 2\mu[\cosh\alpha-\cos 2\mu]^{-1}. \tag{4.12}$$

The obvious advantage of the transformation (4.10) is that the kernel of the integral equation becomes a difference kernel. Thus (4.8′) can be solved by Fourier transforms *provided that* $b=\infty$. But $b=\infty$ corresponds to $Q=\pi-\mu$, which occurs for $n/N=\frac{1}{2}$. Fortunately, this is the case we are interested in; for any other value of n/N, (4.8′) can not be solved analytically.

Returning to our largest eigenvalue in any given n subspace, with n/N fixed, we have, using (3.7), (3.2), and (4.7),

$$\begin{aligned}
&2\lim_{N\to\infty}N^{-1}\ln\Lambda(n/N)\\
&\quad=-\lim_{N\to\infty}N^{-1}\sum_{j=1}^{n}\ln(2-2\cos k_j)\\
&\quad=-\int_{-Q}^{Q}\ln(2-2\cos q)\rho(q)dq\\
&\quad=-\frac{1}{2\pi}\int_{-b}^{b}\ln[1-3(1+2\cosh\alpha)^{-1}]R(\alpha)d\alpha,
\end{aligned} \tag{4.13}$$

the last expression being the result of the transformation (4.10) (with $\cos\mu=-\frac{1}{2}$). Obviously, in (4.13) we have passed from a sum to an integral in the normal way. Strictly speaking, a proof of this step is required, however, because the function $\ln(2-2\cos k)$ has a mild divergence at $k=0$. We are unable to supply the proof at this time, but we hope that the promised paper of YY on the distribution of the k's will enable us to find a proof.

We have purposely left the quantity n/N arbitrary in (4.13) so that we can now give the proof, promised in Sec. II, that Λ is largest for $n/N=\frac{1}{2}$. As n/N decreases from $\frac{1}{2}$, two things happen: (a) The range of integration b decreases monotonically; (b) for any fixed α, the function $R(\alpha)$ decreases monotonically (YY II.13, *et seq.*). Since the integrand in (4.13) is strictly positive we conclude that $\Lambda(n/N)$ is a strictly increasing function for $0\leq n/N\leq\frac{1}{2}$.

For $n/N=\frac{1}{2}$, $b=\infty$ and

$$R(\alpha)=\pi[2\mu\cosh(\pi\alpha/2\mu)]^{-1}, \tag{4.14}$$

(YY II.14a). Thus, from (2.3)

$$\begin{aligned}
2\ln W&=-\frac{3}{8\pi}\int_{-\infty}^{\infty}\frac{d\alpha}{\cosh(3\alpha/4)}\ln\left[1-\frac{3}{1+2\cosh\alpha}\right]\\
&=-\frac{3}{2\pi}\int_{-\infty}^{\infty}\frac{x^2dx}{x^6+1}\ln\left[\frac{(x^2-1)^2(x^2+1)^2}{1+x^4+x^8}\right].
\end{aligned} \tag{4.15}$$

The latter form is obtained by the substitution $e^{\alpha}=x^4$ and then integrating from $-\infty$ to ∞ because the integrand is symmetric.

The function $(x^6+1)^{-1}$ has three poles in the upper half-plane, three in the lower half-plane, and none on the real axis. Thus, if z is a number with $\mathrm{Im}(z)\neq 0$, it is elementary to do the integral

$$\int_{-\infty}^{\infty}x^2dx(x^6+1)^{-1}\ln(x-z)$$

by closing the contour in the half-plane that does not contain z and evaluating the residues at the three poles. Hence, since x^8+x^4+1 and x^2+1 have no zeros on the real axis, it is tedious, but elementary, to deduce

$$\begin{aligned}
&\int_{-\infty}^{\infty}x^2dx(x^6+1)^{-1}\ln(1+x^4+x^8)=\tfrac{2}{3}\pi\ln 8/3.\\
&\int_{-\infty}^{\infty}x^2dx(x^6+1)^{-1}\ln(1+x^2)=\tfrac{2}{3}\pi\ln\tfrac{3}{2}.
\end{aligned} \tag{4.16}$$

The integral involving $\ln(x^2-1)^2$ is trickier, since x^2-1 has zeros on the real axis. We can, however, write

$$\ln(x^2-1)^2=2\,\mathrm{Re}[\ln(x-1)+\ln(x+1)], \tag{4.17}$$

with the logarithmic branches taken to lie on the real axis. Let C be a contour lying above the real axis, but below the poles of $(x^6+1)^{-1}$. If we integrate along C and close the contour in the upper half-plane, we again pick up the residues of $(x^6+1)^{-1}$. Thus,

$$\begin{aligned}
&\int_{-\infty}^{\infty}x^2dx(x^6+1)^{-1}\ln(x^2-1)^2\\
&\quad=2\,\mathrm{Re}\int_{C}x^2dx(x^6+1)^{-1}[\ln(x+1)+\ln(x-1)]\\
&\quad=\tfrac{2}{3}\pi\ln\tfrac{1}{2}.
\end{aligned} \tag{4.18}$$

Inserting (4.16) and (4.18) into (4.15), we obtain the final result

$$W=(\tfrac{4}{3})^{3/2}. \tag{4.19}$$

Note added in proof. Professor Andrew Lenard has informed me (private communication) that the solution to the ice problem is also the solution to the three color problem on a square "map." The problem posed is this: given a finite planar surface composed of squares (the same lattice we have been discussing), in how many ways can the squares be colored with three colors A, B, and C so that adjacent squares never have the same color. Aside from a factor of 3, the two problems are isomorphic. Lenard's solution is to pick one square and color it A (or B or C). Then, for each ice configuration there is a unique coloring and conversely. First arrange

the colors cyclically (i.e., B follows A, C follows B, and A follows C). Consider one of the four vertices surrounding the given A color. This vertex will have two arrows in and two out. The four squares surrounding this vertex are colored uniquely by proceeding clockwise and using the rule that an outward arrow on a bond separating two squares means that the color of the later square follows that of the previous square in the cyclic order given above. Conversely for an inward arrow. After these four squares (one of which is the original A square) have been colored, one proceeds to the next vertex and so on.

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I should like to thank Professor S. Sherman and Dr. J. Nagle, who, in separate conversations, brought this problem to my attention.

APPENDIX: DEPENDENCE OF THE LARGEST EIVENVALUE ON n

While we are mainly interested in proving that the largest eigenvalue lies essentially in the $n=\frac{1}{2}N$ subspace, we will prove here a much broader theorem relating to more general lattices because it will be useful in subsequent work on the solution of Rys's antiferroelectric F model.[8] We want not only to sum over all allowed configurations, but to do so with a weight that is a product of single vertex weights.

Of the 16 *a priori* vertex configurations, the ice condition permits 6. These are shown in Fig. 1. With these we associate energies $e_1,\ldots,e_6$, respectively, and Boltzmann factors $b_j=\exp(-\beta e_j)$. For the ice problem, $b_j=1$ (all j). The partition function is

$$Z=\sum_{\text{allowed configurations}}\prod_{j=1}^{6} b_j^{m_j}, \tag{A1}$$

where m_j is the number of vertices of type j in a configuration.

Again, we can define a transfer matrix $A(\varphi,\varphi')$, but the elements will be different from before. However, (2.6) will still be true, i.e., $A(\varphi,\varphi')=0$ unless the statement preceding (2.6) is satisfied; in particular A still conserves the value of n. We would also like to retain the "up/down" symmetry of the original problem: If ψ is obtained from φ by reversing all spins (V bonds) and if ψ' is likewise related to φ', then $A(\psi,\psi')=A(\varphi,\varphi')$. To obtain this symmetry, it is necessary to reverse all the arrows on the intervening H bonds. Therefore, to retain this symmetry we require

$$b_1=b_2$$

and

$$b_3=b_4$$

and

$$b_5=b_6 \quad \text{for up/down symmetry.} \tag{A2}$$

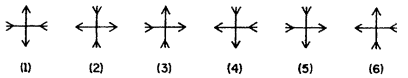

FIG. 1. The six vertex configurations allowed by the "ice condition." The vertex represents an oxygen atom and the arrows indicate on which side of an O-O bond the hydrogen atom lies.

The ice problem also has a "left/right" symmetry: If ψ is obtained from φ by reading backwards (i.e., S_j is replaced by S_{n-j+1}) and if ψ' is likewise related to φ' then $A(\psi,\psi')=A(\varphi,\varphi')$. To retain this symmetry we require

$$b_3=b_6$$

and

$$b_4=b_5 \quad \text{for left/right symmetry.} \tag{A3}$$

For the Rys antiferroelectric F model, the assignments are[8]

$$\begin{aligned} &b_1=b_2=1,\\ &0<b_3=b_4=b_5=b_6<1, \end{aligned} \tag{A4}$$

while for the Slater ferroelectric KDP model the assignments are[8]

$$\begin{aligned} &0<b_1=b_2=b_5=b_6<1,\\ &b_3=b_4=1. \end{aligned} \tag{A5}$$

Thus, both models have up/down symmetry but only the F model has left/right symmetry.

While it appears to be possible to prove the following theorems under the assumption of up/down symmetry alone, we shall, in the present discussion, retain both symmetries. The reason we do so is that left/right symmetry adds a useful simplification, namely, that the transfer matrix A is then real and symmetric: $A(\psi,\psi')=A(\psi',\psi)$. (This is proved by reversing all intervening H bonds.) A virtue of the Hermiticity of A is that the largest eigenvalue can be defined by a variational principle. Without this principle, the proofs below become rather involved and the added complication seems unwarranted at this time.

While we exclude the KDP model, we are prepared to distinguish between ferro- and antiferroelectrics according to the criterion

$$\begin{aligned} &b_3=b_4=b_5=b_6>b_1=b_2 \quad \text{ferroelectric,}\\ &b_3=b_4=b_5=b_6<b_1=b_2 \quad \text{antiferroelectric.} \end{aligned} \tag{A6}$$

In analogy with (2.2), we define $f(n,N)$ by

$$e^{Nf(n,N)}=\Lambda(n,N), \tag{A7}$$

where $\Lambda(n,N)$ is the maximum eigenvalue of Λ in a given n subspace with N columns in the lattice (we retain the original "torus" lattice). By up/down symmetry:

$$f(n,N)=f(N-n,N). \tag{A8}$$

We will prove

Theorem I: Let $n(N)\leq N$ be any sequence of integers such that the limit

$$\rho=\lim_{N\to\infty} n(N)/N \tag{A9}$$

exists. Then: (a) the limit $f(n(N),N)$ exists, is a function only of ρ, and is continuous, i.e.,

$$F(\rho)=\lim_{N\to\infty} f(n(N),N); \tag{A10}$$

(b) $F(\rho)$ is concave, i.e., for $0\leq\rho_1,\rho_2\leq 1$,

$$F(\tfrac{1}{2}(\rho_1+\rho_2))>\tfrac{1}{2}[F(\rho_1)+F(\rho_2)]. \tag{A11}$$

Corollary 1. By (A8)

$$F(\rho)=F(1-\rho). \tag{A12}$$

Corollary 2.

$$\max_{\rho} F(\rho)=F(\tfrac{1}{2}). \tag{A13}$$

Corollary 3. Let $n(N)$ be a maximal sequence, i.e., for each N

$$g(N)\equiv f(n(N),N)\geq f(n,N), \quad (\text{all } 0\leq n\leq N). \tag{A14}$$

Then g has a limit and

$$\lim_{N\to\infty} g(N)=F(\tfrac{1}{2}). \tag{A15}$$

Proof: Since $n(N)$ is maximal, we have by (A10) and (A13) that $\lim_{N\to\infty}\inf g(N)\geq F(\frac{1}{2})$. Suppose $\lim_{N\to\infty}\sup g(N)>F(\frac{1}{2})$. Then we can find an infinite subsequence, $(N_{\alpha 1},N_{\alpha 2},\ldots)$ such that for some $\epsilon>0$ $g(N_{\alpha j})>F(\frac{1}{2})+\epsilon(\text{all } j)$. Define $\rho_{\alpha j}\equiv n(N_{\alpha j})/N_{\alpha j}$. There must be at least one point of accumulation, call it ρ. Then we can find an infinite subsequence $(N_{\beta 1},N_{\beta 2},\ldots)$ of the first subsequence such that

$$\lim_{j\to\infty}\rho_{\beta j}=\rho.$$

By (A13),

$$\lim_{j\to\infty} g(N_{\beta j})\leq F(\tfrac{1}{2}),$$

which is a contradiction. Hence

$$F(\tfrac{1}{2})=\lim_{N\to\infty}\sup g\geq\lim_{N\to\infty}\inf g\geq F(\tfrac{1}{2}). \quad \text{Q.E.D.}$$

Obviously, Corollary 3 is what we needed for our ice calculation.

Proof of Theorem I. (a) As before, when $\varphi=\varphi'$ there are two choices for the intervening H bonds, whereas when $\varphi\neq\varphi'$ there is at most one choice. The diagonal part A_D depends only on n and N:

$$\begin{aligned}A_D=A(\varphi,\varphi)&=(b_5)^n(b_3)^{N-n}+(b_4)^n(b_6)^{N-n}\\&=(b_5)^n(b_3)^{N-n}+(b_3)^n(b_5)^{N-n}.\end{aligned} \tag{A16}$$

As $N\to\infty$, A_D has a limit as in the theorem, i.e., (for $b_3\geq b_5$),

$$\begin{aligned}\lim_{N\to\infty} N^{-1}\ln A_D&=F_D(\rho)\\&=\tfrac{1}{2}\ln(b_3b_5)+|\tfrac{1}{2}-\rho|\ln(b_3/b_5),\end{aligned} \tag{A17}$$

but this is a *convex* function. [Note: in (A17) we used only up/down symmetry.] (b) Write

$$A(\varphi,\varphi')=A_D\delta(\varphi,\varphi')+A_L(\varphi,\varphi')+A_R(\varphi,\varphi'),$$

where A_L is the off-diagonal part that produces exchanges $-+$, $+-$, etc., when reading from left to right; A_R is the opposite. Henceforth, assume $n\leq\frac{1}{2}N$. An antiferroelectric upper bound for A_L+A_R is obtained by noticing that there can be at most $2n$ vertices of type (1) or (2). Hence $A_L+A_R\leq(b_1)^{2n}(b_3)^{N-2n}$. A ferroelectric upper bound is $(b_3)^N$. Since there are $\binom{N}{n}$ states in the subspace we have the upper bound

$$\Lambda(n,N)\leq A_D+(b_1)^{2n}(b_3)^{N-2n}\binom{N}{n}, \quad \text{antiferroelectric,} \tag{A18a}$$

$$\leq A_D+(b_3)^N\binom{N}{n}, \quad \text{ferroelectric.} \tag{A18b}$$

A lower bound for Λ can be obtained by the variational function (here we use left/right symmetry in order that A be Hermitian)

$\psi=2^{-1/2}(\varphi_1+\varphi_2)$. For antiferroelectrics:

$$\varphi_1=(\overbrace{+-\cdots+-}^{2n}\ \overbrace{++++\cdots+}^{N-2n})$$

and

$$\varphi_2=(\overbrace{-+\cdots-+}^{2n}\ \overbrace{++++\cdots+}^{N-2n}).$$

Thus,

$$\Lambda(n,N)\geq\tfrac{1}{2}(b_1)^{2n}(b_3)^{N-2n} \quad \text{(antiferroelectric).} \tag{A19a}$$

For ferroelectrics:

$$\varphi_1=(\overbrace{-+\cdots++}^{N-n}\ \overbrace{--\cdots-}^{n-1})$$

and

$$\varphi_2=(\overbrace{+++\cdots+}^{N-n}\ \overbrace{---\cdots-}^{n}).$$

Thus,

$$\Lambda(n,N)\geq\tfrac{1}{2}b_1{}^2b_3{}^{N-2} \quad \text{(ferroelectric).} \tag{A19b}$$

Note that in both cases the lower bound was obtained from A_L+A_R without A_D.

(c) If $\rho=0$, then as $N\to\infty$, (A17) and (A19) agree and we have proved the theorem with

$$F(0)=F_D(0)=\ln b_3. \tag{A20}$$

If $\rho>0$, we see that the lower bound (A19) (which came from A_L+A_R) approaches a limit that is greater than or equal to $F_D(\rho)$. Hence, we shall drop A_D and consider only $A'=A_L+A_R$.

(d) For $\rho>0$, we need consider only $\Lambda'(n,N)=$ largest eigenvalue of A_L+A_R. A useful characterization of Λ' is the following: Define

$$\Lambda_L(n,N)\equiv\max_\Psi(\Psi,A_L\Psi)/(\Psi,\Psi)\,, \qquad \text{(A21a)}$$

where Ψ is restricted to the n subspace and is real. Since the Euler-Lagrange equation for Λ_L is $\frac{1}{2}(A_L+A_L^{\dagger})\Psi=\Lambda_L\Psi$, and since $A_L^{\dagger}=A_R$ (here we use left/right symmetry), it is a trivial conclusion that

$$\Lambda_L(n,N)=\tfrac{1}{2}\Lambda'(n,N)\,. \qquad \text{(A21b)}$$

Define $f_L(n,N)$ in analogy with (A7) using Λ_L. Since the factor $\frac{1}{2}$ in (A21b) is irrelevant as $N\to\infty$, we have

$$F(\rho)=F_L(\rho)\,, \qquad \text{(A22)}$$

assuming that we can prove that f_L satisfies theorem I.

(e) To prove Theorem I for f_L, we shall utilize a method that is by now almost classic.[11] Let $\Psi(n,N)$ be the function that maximizes $\Lambda_L(n,N)$. Divide the chain (row) into two pieces with N_1 vertices in the first part, N_2 in the second, and $N_1+N_2=N$. In an obvious notation, consider the following trial function for the full chain $\bar{\Psi}(n,N)=\Psi(n_1,N_1)\Psi(n_2,N_2)$, with $n_1+n_2=n$. The reason for considering Λ_L alone now becomes apparent, for

$$(\bar{\Psi},A_L\bar{\Psi})/(\bar{\Psi},\bar{\Psi})=\Lambda_L(n_1,N_1)\Lambda_L(n_2,N_2)\,. \qquad \text{(A23)}$$

The proof of (A23) follows from the observation that the only part of A_L which contributes to $(\bar{\Psi},A_L\bar{\Psi})$ is that part which conserves both n_1 and n_2 separately. Also, when we go from the broken chain to the full chain we must add the H bond connecting N_1 to N_1+1 and N to 1. But we must also delete the H bonds connecting N_1 to 1 and N to N_1+1. The crux of the matter is that for those terms in $(\bar{\Psi},A_L\bar{\Psi})$ that do not vanish, the arrows along the two added H bonds are exactly the same as they would be along the two deleted H bonds of the broken chain. If we now define $g(\rho,N)=f_L(n,N)$ with $\rho=n/N$, we have from (A23)

$$g(\rho,N)\geq\omega_1 g(\rho_1,N_1)+\omega_2 g(\rho_2,N_2)\,, \qquad \text{(A24)}$$

with $\omega_j=N_j/N$ and $\rho=\omega_1\rho_1+\omega_2\rho_2$. We can define g for nonintegral values of n by linear interpolation: If $\rho=(n+\eta)/N$ with $0\leq\eta\leq1$, then

$$g(\rho,N)\equiv(1-\eta)g(n/N,N)+\eta g((n+1)/N,N)\,. \qquad \text{(A25)}$$

With this definition, it is possible to show that (A24) is *a fortiori* true for arbitrary ρ_1 and ρ_2 (cf. Ref. 11, footnote 25).

(f) From (A18) and (A19), we have the following large N bounds on g (valid for $\rho\neq0$, i.e., $n\neq0$): For antiferroelectrics

$$g(\rho,N)\leq\rho\ln[b_1^2(1-\rho)/b_3^2\rho]+\ln[b_3/(1-\rho)]\,,$$
$$g(\rho,N)\geq2\rho\ln[b_1/b_3]+\ln b_3\,. \qquad \text{(A26a)}$$

For ferroelectrics

$$g(\rho,N)\leq\rho\ln[(1-\rho)/\rho]+\ln[b_3/(1-\rho)]\,,$$
$$g(\rho,N)\geq\ln b_3\,. \qquad \text{(A26b)}$$

(g) Pick some $N_0>0$ and consider the sequence $N_j=2^jN_0$ with ρ fixed. Define $g_j\equiv g(\rho,N_j)$. Then (A24) states that g_j forms an increasing sequence. Since it has an upper bound (A26), it must have a limit. Call this limit $G(\rho,N_0)$. Now set $N_1=N_2=N_02^j$ and $N=2N_02^j$ in (A24) and take the limit $j\to\infty$. We thereby establish the concavity of $G(\rho,N_0)$. This function is, moreover, continuous, since a concave function bounded from below is necessarily continuous.

(h) We now wish to show that $G(\rho,N_0)$ is the common limit for an arbitrary sequence $\rho(N)=n(N)/N$ satisfying the conditions of the theorem. This will be done by showing that $\lim_{N\to\infty}\inf g(\rho(N),N)\geq G(\rho,N_0)$ and $\lim_{N\to\infty}\sup g(\rho(N),N)\leq G(\rho,N_0)$.

Lower bound: Obviously, the inequality (A24) can be iterated any number of times. In particular, let j be fixed and let $L=N_02^j$. Break the chain up into C subchains of length L plus a remainder of length M ($CL\leq N$ and $M=N-CL$). Then

$$g(\rho(N),N)\geq(CL/N)g(\rho,L)+(1-CL/N)g(\rho',N-CL)\,, \qquad \text{(A27)}$$

with $\rho'=[N\rho(N)-\rho CL][N-CL]^{-1}$. We wish to insure that $0<\rho'\leq\frac{1}{2}$, which means that $CL/N\leq[\frac{1}{2}-\rho(N)]\times[\frac{1}{2}-\rho]^{-1}$ and $CL/N<\rho(N)/\rho$. If C is always chosen to be the maximum integer satisfying these requirements then, as $N\to\infty$, $1-CL/N\to0$. But $g(\rho',N-CL)$ is bounded by (A18). Thus, letting $N\to\infty$ in (A27) yields $\lim_{N\to\infty}\inf g(\rho(N),N)\geq g(\rho,L)$. This is true for all j. Now let $j\to\infty$, whence $\lim_{N\to\infty}\inf g(\rho(N),N)\geq G(\rho,N_0)$.

Upper bound: L is defined as above. For each N let k be the smallest integer such that $U=N_02^k\geq2N$. Consider a chain of length U broken up into a piece of length N, C pieces of length L and a remainder of length $M=U-N-CL$. Then (A24) states that

$$g(\rho,U)\geq(N/U)g(\rho(N),N)+(CL/U)g(\rho,L)+(M/U)g(\rho',M)\,,$$

where $\rho'=[\rho U-\rho CL-N\rho(N)][U-CL]^{-1}$. In order to have $0<\rho'\leq\frac{1}{2}$ we require $CL/U<1-N\rho(N)/U\rho$. If C is the maximum possible integer for each N then, as $N\to\infty$, $U^{-1}(N+CL)\to1$. Therefore, $(M/U)g(\rho',M)\to0$. Hence

$$\limsup_{N\to\infty}g(\rho(N),N)\leq\lim_{N\to\infty}g(\rho,U)+(-1+U/N)g(\rho,U)$$
$$-(CL/N)g(\rho,L)\leq G(\rho,N_0)+3|G(\rho,N_0)-g(\rho,L)|\,.$$

(We have used the fact that $U/N<4$.) Now let $j\to\infty$, so that the last quantity, $|\ |$, goes to zero. Q.E.D.

[11] See, for example, M. E. Fisher, Arch. Rat. Mech. Analysis 17, 377 (1964). It is to this paper that we are most indebted.

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Two-Dimensional Ferroelectric Models

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The two-dimensional ferroelectric configuration is an array of arrows drawn on the bonds of a usual square lattice, one arrow for each bond. The *ice constraint* (I.C.) is that precisely two arrows point into and two point out of each vertex of the lattice. A lattice with N vertices has $2N$ bonds, so that without the ice constraint there are $Z=2^{2N}$ configurations. It has been shown recently[1] that asymptotically the number of configurations is given by $\lim_{N\to\infty} N^{-1} \ln Z=\left(\frac{4}{3}\right)^{3/2}$.

It will be seen that the I.C. permits a total of 6 possible arrow configurations in the neighborhood of each vertex, as distinguished from the unrestricted number of 16. These 6 are naturally divided into two types: *Type* 1: In these the arrows go "straight through" the vertex. There are 4 of these and they each have a net polarization in one of 4 directions; *Type* 2: In these the arrows oppose each other. There are 2 of these and they have no polarization.

In the ferroelectric models we associate an energy to each kind of vertex and hence, by simple addition, to an entire configuration. There are two basic types of models: *F Models* (Rys 1963): Type 1 vertices have an energy $\varepsilon>0$ while Type 2 vertices have zero energy. This is a model of an antiferroelectric because polarization is discouraged. The ordered state is one in which the two Type 2 vertices alternate on the lattice. *KDP Model* (Slater 1941): Here one pair of vertices of Type 1 with opposite polarization are preferred by having zero energy. The rest have energy $\varepsilon>0$. This is a model of a ferroelectric because the ordered state has perfect polarization.

By a straightforward, but not entirely trivial generalization of the method used to enumerate the number of ice configurations the partition function for the ferroelectric models can be found.[2] In fact it can also be found when an arbitrary external electric field is present along one of the principal directions.

Some of the main physical properties of these models are listed below. Many of them have not been previously reported in the literature and much of this work has been done in collaboration with Dr. F. Y. Wu.

With E=electric field=0 both models have the same critical temperature, T_c, given by

$$T_c(E=0)=T_0\equiv\varepsilon\{k \ln 2\}^{-1} . \qquad (1)$$

For both models, T_c depends on electric field, but in quite different ways and with different critical point properties. To study the properties of these systems it is convenient to discuss the free energy, F, as a function of y=average polarization/vertex. It is given by

$$F(T, E, y)=G_T(y)-Ey , \qquad (2)$$

where G is the free energy in the absence of electric field. The value of y is that which minimizes eq. (2). G is, of course, symmetric and convex upwards in y for fixed T, and decreases with increasing T for fixed y.

KDP: For $T\leq T_0$, $G=0$ for all y. Hence, $C\equiv$ specific heat=0 and an infinitesimal E produces perfect polarization. The internal energy $\equiv U=-E$. For $T\geq T_0$, G appears like a nested sequence of parabolas with the common value $G=0$ at $y=\pm 1$. These flatten out as $T\to T_0$. For all finite T the slope at $y=\pm 1$ is finite which implies that a finite E can produce perfect polarization. For $E=0$ we move up the $y=0$ axis as T decreases until we reach the point $G=0$, $y=0$ when $T=T_0$. There is a singularity at this point having the following physical consequences at T_0: (1) U is discontinuous (first order phase transition); (2) C goes to infinity on the high T side like $(T-T_0)^{-1/2}$.

When $E>0$, $y=0$ at $T=\infty$ and increases as T decreases. Since the slope of G at $y=1$ is finite, the point $y=1$ is reached for some temperature $T_c(E)>T_0$. Thereafter y sticks at 1. The physical consequences of this are: (1) Unlike the ferromagnetic Ising model, the critical point does not disappear with an applied field. Rather, $T_c(E)$ is an increasing function of E, approaching ∞ at $E=\infty$; (2) For $E>0$ the critical point is at $y=1$ which is far removed from $y=0$. The latent heat disappears (*i.e.* the transition becomes second order), but C continues to have the same critical exponent as before, although with a different residue.

When y is eliminated from eq. (2) we can study

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F in the (T, E) plane. For $E>0$ there is a critical line $T_c(E)$ extending from $(T_0, 0)$ outwards to (∞, ∞). R. Griffiths has suggested (privately) that the scaling hypothesis would imply that the function F, in two similar nested neighborhoods about $(T_0, 0)$, should scale according to some power law. Unfortunately, this is not the case, for, as the above discussion would suggest, and as can be indeed verified, F scales differently along the $E=0$ axis than it does along the $T_c(E)$ curve, however close one approaches $(T_0, 0)$. In this sense the scaling law is violated for KDP. If, however, we investigate the neighborhood of some other point along the critical line, *i.e.* $(T_c(E), E)$, then scaling is valid.

F Model: For $T>T_0$ the $G_T(y)$ curves look qualitatively similar to those for KDP, except that the slope at $y=\pm 1$ is infinite. This implies that an infinite E is required for perfect polarization. Another difference from KDP is that the curves become more convex, rather than less, as T is decreased. In fact, below T_0 the curves have a non zero, discontinuous derivative at $y=0$ (a cusp). Hence, below T_0 a non zero field, $E_c(T)$, is required to produce any polarization at all. When $E=0$ the point $T=T_0$, $y=0$ is singular. This gives rise to an infinite order phase transition, *i.e.* $\partial^n G_T(0)/\partial T^n$ is bounded and continuous at T_0, for all n, but no power series expansion is possible at T_0. When $E\neq 0$, y at first increases as T is decreased from ∞, but then begins to decrease, finally reaching zero at some $T_c(E)<T_0$. $T_c(E)$ decreases with E and reaches zero (*i.e.* the transition disappears) when $E=\varepsilon$. For $T<T_c(E)$ we again follow the $y=0$ axis, which means that below $T_c(E)$ all thermodynamic quantities are exactly the same as for $E=0$. Because y approaches zero with a discontinuous slope at $T_c(E)$, C turns out to have an infinity on the high T side which behaves like $\{T-T_c(E)\}^{-1/2}$. There is no latent heat, however, so that a non zero E produces a second order phase transition.

An unsolved problem is to test the scaling hypothesis for the F model. To do so, we have to apply a staggered quadrupole field (introduced by J. Nagle) which interacts only with the two vertices of type 2.

Another interesting unsolved problem (suggested by I. Syozi) is to solve these models for the Kagome lattice which also has a coordination number of four.

A variant of these models that *can* be solved is the ferrielectric model. This is similar to KDP except that the favored type 1 vertices are chosen to alternate from row to row. Although there is no 1:1 configurational correspondence with KDP, the thermodynamics of this model is exactly the same as for KDP even with $E\neq 0$, provided E is in the vertical direction.

Two other important unsolved problems are:
(1) To allow two other vertices, namely those with 4 arrows in and 4 out, but with arbitrary energy of course. The Ising model with crossed bonds is equivalent to a special case of this.
(2) The number of ice configurations is easily seen to be the same as the number of 3-colorings of an infinite map of square countries. Can one do the 4 or, in general, the k-coloring problem?

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Relations between the 'percolation' and 'colouring' problem and other graph-theoretical problems associated with regular planar lattices: some exact results for the 'percolation' problem

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A transfer-matrix approach is introduced to calculate the 'Whitney polynomial' of a planar lattice, which is a generalization of the 'percolation' and 'colouring' problems. This new approach turns out to be equivalent to calculating eigenvalues and traces of Heisenberg type operators on an auxiliary lattice which are very closely related to problems of 'ice' or 'hydrogen-bond' type that have been solved analytically by Lieb (1967*a* to *d*). Solutions for certain limiting cases are already known. The expected numbers of components and circuits can now be calculated for the plane square lattice 'percolation' problem in a special class of cases, namely those for which $p_H + p_V = 1$ where p_H and p_V are, respectively, the probabilities that any given horizontal or vertical bond is present. This class of cases is known, from the work of Sykes & Essam (1964, 1966), to be critical in the sense that a connected path across a large lattice exists with probability effectively unity whenever $p_H + p_V \geqslant 1$. Relations with other problems involving the enumeration of graphs on lattices, such as the tree, Onsager and dimer problems are pointed out. It is found that, for the plane square lattice, the treatment of problems of 'ice' type is very considerably simplified by building up the lattice diagonally, rather than horizontally or vertically.

The two available analytic methods of handling these problems, the Bethe–Húlthen 'ansatz' approach and the Kaufman–Onsager 'spinor' approach are compared.

1. Introduction

A very wide variety of physical and technical problems associated with repeating networks or crystals can be reduced to graph-theoretical form, involving enumerations of arrangements of points and lines on a lattice subject to certain restrictions. Throughout this paper, the word 'lattice' is used in the physical and not in the mathematical sense and we shall use the regular plane square lattice, in which each 'point' or 'node' or 'site' is connected by 'lines' or 'bonds' to four nearest neighbouring points, by way of illustration. (Unless otherwise stated, the word 'line' or 'bond' refers to one connecting a pair of nearest neighbouring points of the lattice.) By a 'graph' we mean a collection of such lines, together with the points that they intersect and any remaining isolated points of the lattice. A 'subgraph' is obtained from a graph by deleting one or more of its lines *without* removing any of the points. A 'component' (of a graph or subgraph) is a maximal connected portion of the

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graph. The words 'circuit' and 'tree' have their usual meanings, a 'forest' is a collection of disconnected trees and isolated points. It will be assumed that the reader is familiar with Euler's notion of independent circuits. The 'cyclomatic number' or 'nullity' of any graph or component is the number of independent circuits in it. We shall often imagine the lattice to be progressively built up row by row, neighbouring points in a row being added one at a time, and we shall then use the expression 'lattice' as an abbreviation for 'the graph consisting of all the points added so far, together with all the nearest neighbour bonds between pairs of these points'. We do not postulate the addition of a line to a graph unless both its end-points have already been added to the lattice.

In some problems we shall be concerned with directed lines and we shall denote these by arrows or by positive or negative signs, but we shall never introduce multiple lines between a pair of points. We shall also recognize the possibility that points on the lattice may be 'coloured' in two or more different ways.

2. Types of problem of physical interest

It is obvious that a very large number of mathematical problems can be posed about arrangements of points and lines on a lattice. In this paper we shall be concerned with relations between four types of problem of physical interest.

A. The enumeration of trees and forests is possible for any lattice, planar or not, the general theory having been laid down by Kirchoff and Sylvester. More complicated problems, however, arise if individual trees are to be weighted according to certain prescriptions. See, for example, Tutte (1954).

B. The enumeration of the number of ways of disposing $\frac{1}{2}$L black points on a plane square lattice of L points with a specified number of nearest-neighbour black pairs was accomplished by Onsager (1944). The results, which are of considerable interest in a number of branches of physics, for example magnetism, metallurgy, theory of solutions, adsorption, have since been extended to virtually all regular planar lattices and have been re-derived by a variety of different methods, but with only marginal improvements on the scope of Onsager's original results. (For example, a little is now known about arrangements involving three or four colours (Betts 1964) and about correlations at various distances (Kaufman & Onsager 1949).)

C. Recently Lieb (1967*a* to *d*) and others have given a unified treatment of a set of physical problems of 'hydrogen-bond' or 'ice' type. The simplest such problem is to ask for the number of ways in which arrows can be assigned to bonds on the lattice, in such a way that exactly two arrows point to every node. This models the situation for hydrogen-bonded molecules. In ice, for example, each hydrogen atom can occupy one of two positions between a pair of oxygen atoms, but, in the neighbourhood of each oxygen there are always the same numbers of hydrogens in the 'near' and 'distant' positions. These numbers are obviously two each if we 'model' ice by putting oxygens on the points of a plane square lattice, the hydrogens each occupying one of the bonds in two possible positions subject to the above. There are

six types of node, 1 to 6 of figure 1, satisfying the above restriction. More sophisticated problems of this type, in which different statistical mechanical probabilities are assigned to the six types of node satisfying the ice condition have also been solved; Lieb (1967*b*, *c*), Sutherland (1967), Sutherland, Yang & Yang (1967), Yang (1967). These serve as models of ferroelectric and antiferroelectric assemblies, with or without an applied electric field.

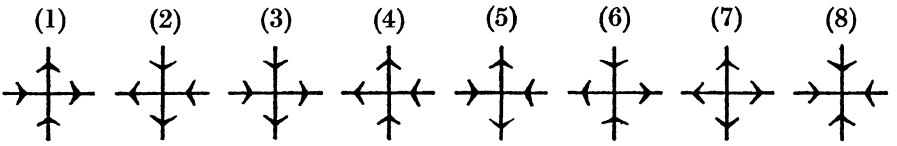

FIGURE 1

D. The problem of the number of ways of colouring the points of a lattice with k colours in such a way that no two neighbouring points are coloured alike was studied and generalized by Whitney (1932). The problem is trivial for $k = 1$ or 2. For $k = 3$ the problem on the plane square lattice is equivalent to the ice problem (Lieb 1967*d*). No other exact result is known at present. Whitney's generalization turned out to be closely related to the 'percolation' problem, which amounts to asking for the expected number of connected components of a random graph, each bond on the lattice having a chance p or $1-p$ of being selected or rejected for inclusion in the graph. This is closely connected with various problems in magnetism and is also of interest in communication and porous medium problems, when we think of each bond as being 'open' or 'blocked' and ask for the probability that a continuous path exists through the whole lattice. Sykes & Essam (1964, 1966) rediscovered a result of Whitney (1932), a dual transformation very similar to that known to exist for the Onsager (1944) problem, and were able, for several lattices, to determine the critical value of p above which a long path through the lattice (or equivalently, a large connected domain of 'open' bonds), might be expected to occur with a probability of effectively unity. This was a very important piece of information, but left outstanding the more general problem, namely that of determining in general the number of ways of choosing M lines which have points in common in such a way as to give rise to N disconnected components. (Obviously there are two different versions of the problem according to whether or not we count an isolated point in the lattice, not intersected by any of the M lines, as a 'component' of the graph.) The related 'dimer' problem (Kasteleyn 1962; Temperley & Fisher 1961), in which we ask for the number of ways of choosing $\frac{1}{2}$L lines from a lattice of L points in such a way that no two of them pass through the same point on the lattice, so that there are no isolated points and $\frac{1}{2}$L components each consisting of one line, can be solved (by a variety of methods) for any regular planar lattice, but it is only for this limiting case that an analytic solution is known at present. (In graph-theoretical terminology this problem amounts to determining the number of 1-factors of a lattice.)

3. General relations between these problems

We shall interest ourselves only in the analytic form of the solutions of these problems in the limiting case where L, the number of points on the lattice, is very large. A very considerable amount of information about all these problems is also available from series expansions of various types, obtained by direct enumeration of configurations involving relatively small numbers of points and lines, followed by attempts to deduce trends for large graphs. In this paper we shall make only one comparison with this approach. We are far from attempting to deny its utility. Indeed, until quite recently, the number of analytic results available was quite small, and it is enough to say that, in all cases where comparison of series and analytic results has been possible, agreement has been very close indeed.

Lieb (1967*a* to *d*) showed that there is a very close analytical connexion between problems of 'generalized ice' type (type C above) and another problem that has an extensive literature, namely a one-dimensional array of 'spins' each interacting with two nearest neighbours with a Heisenberg type interaction. He was able to exploit various known results about this one-dimensional array and to obtain exact solutions for the various 'generalized ice' problems.

In this paper we shall do two things. We shall exhibit the relationships between these types of problem in a new and physically more transparent light. We shall also derive a transfer-matrix approach to Whitney's (1932) problem (generalization of the percolation and chromatic polynomial problems), and we shall show that this problem, too, can be reduced to problems of 'generalized ice' type which might be soluble by similar means. Various relations with Tutte's work (1954) on the Whitney problem and with the Onsager problem (1944) will also be exhibited, and we shall show how to calculate the expected numbers of components and circuits for the critical cases of the 'percolation' problem.

4. Analytic methods available

Much confusion exists in the literature about notation. One can work with Pauli, Fermi, Heisenberg or permutation operators or with creation and annihilation operators. Throughout this paper we shall use Onsager's (1944) definitions and notation. We describe our assembly by a set of 'spin variables', μ_i, each of which assumes only the values ± 1, and for each spin the operators C_i, S_i have the properties: $C_i 1 \to 1$, $C_i \mu_i \to -\mu_i$, $S_i 1 \to \mu_i$, $S_i \mu_i \to 1$. Since $\mu_i^2 = 1$ we are never concerned with powers of μ_i higher than the first, and the two possible 'states' of 'spin' i are represented by $\frac{1}{2}(1+\mu_i)$ and $\frac{1}{2}(1-\mu_i)$. We can represent C_i and S_i as direct products of 2×2 matrices of Pauli type thus

$$C_i = \mathrm{I} \times \mathrm{I} \times \ldots \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \times \mathrm{I} \times \ldots,$$

$$S_i = \mathrm{I} \times \mathrm{I} \times \ldots \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \times \mathrm{I} \times \ldots.$$

The Onsager interaction operator is $\exp(HS_1S_2)$ and it will be seen that it has the effect of multiplying a term like $\frac{1}{4}(1+\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1-\mu_1)(1-\mu_2)$ by e^H, and any term of the form $\frac{1}{4}(1-\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1+\mu_1)(1-\mu_2)$ by e^{-H}, thus distinguishing between pairs of like and unlike neighbours, in the same row.

The Heisenberg interaction operator can be written

$$C_1C_2 - C_1C_2S_1S_2 + \Delta S_1S_2. \tag{1}$$

If two neighbouring spins are alike, it simply multiplies the term $\frac{1}{4}(1+\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1-\mu_1)(1-\mu_2)$ by Δ. If they are unlike it has the effect

$$\tfrac{1}{4}(1+\mu_1)(1-\mu_2) \to \tfrac{1}{2}(1-\mu_1)(1+\mu_2) - \tfrac{1}{4}\Delta(1+\mu_1)(1-\mu_2). \tag{2}$$

For $\Delta = 1$, it can be simply expressed as $2\mathrm{T}_{12}-1$ where T_{12} is the operator that changes μ_1 into μ_2 and vice versa. This is usually known as the isotropic Heisenberg case. (Note that all operators are to act on quantities appearing to their right, never to their left. Therefore we make the convention that BA is to be interpreted as: First operation A, then operation B.)

Although many variants of them exist in the literature there are, in effect, only two basic methods of tackling these problems. We can express Onsager's operators in terms of anti-commuting 'spinors' in various ways, for example

$$\left.\begin{aligned} S_1 &= P_1 & S_1C_1 &= Q_1 \\ S_2C_1 &= P_2 & S_2C_2C_1 &= Q_2, \\ S_3C_1C_2 &= P_3 & S_3C_3C_2C_1 &= Q_3, \end{aligned}\right\} \tag{3}$$

etc.

so that

$$\left.\begin{aligned} C_1 &= P_1Q_1 & S_1S_2 &= -P_2Q_1 & C_1C_2S_1S_2 &= -P_1Q_2, \\ C_2 &= P_2Q_2 & S_2S_3 &= -P_3Q_2 & C_2C_3S_2S_3 &= -P_2Q_3, \\ &\cdots & &\cdots & &\cdots, \end{aligned}\right\} \tag{4}$$

and, for any problem that be expressed as that of finding the trace of a product like

$$\mathrm{tr}\exp(AP_1Q_1) \times \exp(BP_2Q_1) \times \exp(CP_2Q_2) \times \exp(DP_3Q_2) \times \ldots, \tag{5}$$

in which we have exponentials of second-order products of these spinors, we can exploit the isomorphism of the spinor and rotation groups (Kaufman & Onsager 1949) to infer the eigenvalues and hence the trace. Various other approaches, using determinants, vacuum to vacuum expectations, Wick's theorem, Pfaffians etc. are all nearly equivalent and apply to the same types of case.

For the 'ice-like' problems, the 'ansatz' method introduced by Bethe (1931) exploits the fact that, while the Heisenberg operators (1) may introduce numerical factors, none of them ever changes the total number of plus or minus spins in a row of spins. At most, it permutes pairs of unlike spins, changing $(+\ -)$ to $(-\ +)$. It is this property of a sum (or product) of Heisenberg operators that makes possible the methods used by Bethe (1931) and Húlthen (1938) and a large number of later workers for electron assemblies and applied by Lieb (1967 *a* to *d*) to the 'ice-like' problems.

5. A transfer matrix for the Whitney and percolation problems

The principle of the transfer-matrix is now well known as a result of Onsager's (1944) and other work. Imagine the lattice built up row by row and point by point. In the Onsager model (1944) the interactions are between nearest neighbours only. Then, if (figure 2) we add to the lattice a point such as D', the spin on it interacts with those on points C' and D, but with no others. At each stage we keep, in terms of the μ's, a record of *all* the possible configurations of the spins on all the 'outside' points (that is to say of $A', B', C', D', E, F, \ldots$, at the stage shown in figure 2) each

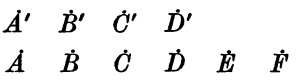

FIGURE 2

configuration weighted with the appropriate Boltzman factor due to the interactions. (These 'outside' points are nearest neighbours of points that will be added at a later stage. We call all other points such as A, B, C 'inside' points, and we need not specify the configuration of their spins.) In terms of the μ's our generating function will contain two sets of terms one corresponding to μ_D being negative, the other to μ_D being positive. These may be written

$$\phi = \tfrac{1}{2}(1-\mu_D) f(\mu'_A, \mu'_B, \mu'_C, \mu_E, \mu_F) + \tfrac{1}{2}(1+\mu_D)\, g(\mu'_A, \mu'_B, \mu'_C, \mu_E, \mu_F).$$

Apply the operator $\exp(HS_D S'_D)$ which gives a factor e^H for a like pair, e^{-H} for an unlike pair and sum over both configurations ($\mu_D = \pm 1$) of spin D that is now on an 'inside' point. The relation between the generating functions before and after adding point D' and putting in the effect of the interaction $(D - D')$ is

$$\phi'(\mu'_A, \mu'_B, \mu'_C, \mu'_D \ldots) = (e^H + C_D e^{-H})\, \phi(\mu'_A, \mu'_B, \mu'_C, \mu_D, \ldots).$$

The interaction $(C' - D')$ can be taken care of simply by operating with $\exp(HS'_C S'_D)$. No summation is performed, since C' and D' are both still 'outside' points. The total effect of adding point D', summing over both configurations of the spin on point D and then allowing for the factor in the partition function due to the interaction $(C' - D')$ is precisely given by operating on ϕ with

$$\exp(HS'_C S'_D)\,(e^H + C_D e^{-H})$$

and we get a similar pair of factors each time we add a point to the lattice. Operators like C_A, $S_B S_C$ are all expressible as quadratic products of spinors as shown by (3) and (4), hence the Onsager problem is soluble.

These considerations are well known, but we have set them down because they give a clue on how to set up the transfer operator for the Whitney problem. Whitney (1932) defined a polynomial for any lattice (which need not be regular)

$$W(x, y) = \sum_G x^{rG} y^{sG}, \tag{6}$$

where G runs over all subgraphs of the lattice, including the null graph and multi-component subgraphs. r_G and s_G are respectively the rank and nullity of G. The nullity of G is defined as the number of independent circuits in G (independent in Euler's sense). The rank is best defined indirectly. If we add a line to a subgraph G in such a way as to connect two points already joined in G we form a new circuit, and the rank is unchanged. Otherwise it is increased by one by adding a line. Thus r_G+s_G is simply the total number of lines in G, Euler's relation then gives the number of components of G as $\mathrm{L}-r_G$, if we make the convention that each isolated point counts as a 'component' of G.

It must now be shown that the chromatic polynomial and the generating function for the number of disconnected components in a random graph on the lattice are both particular cases of (6). The result for the latter is immediate. For a lattice of L points, the number of disconnected components is $\mathrm{L}-r_G$, and since the total number of lines in G, l_G, is just r_G+s_G, we have

$$\sum_G r_G x^{l_G} = \left[x\frac{\partial}{\partial x}W(x,y)\right]_{y=x}. \tag{6a}$$

Dividing this expression by $W(x,x)$ gives us the expected rank (L minus the expected number of components) of a random graph, if we put $p = x/(1+x)$. This is one of the problems of 'bond' type studied by Sykes & Essam (1964, 1966).

To derive the chromatic polynomial, we use the inclusion–exclusion method, following Whitney (1932). The number of ways of colouring the lattice in k colours without restriction is just k^{L}. From this we subtract the number of ways of colouring it so that at least two nearest neighbours are coloured alike, which is $k^{\mathrm{L}-1}\times$ (the number of lines in the lattice). We have now subtracted twice over the number of ways in which the points on a subgraph of type ⌊ are coloured alike which we correct for by adding $k^{\mathrm{L}-2}$ for each subgraph. We make similar corrections for larger subgraphs. When the graph contains circuits the argument becomes more elaborate, and the reader is referred to Whitney's (1932) paper for details, but the final result is

$$p(k) = k^{\mathrm{L}}\mathrm{W}(-1/k, -1). \tag{6b}$$

This asserts that there is a (1–1) correspondence between the terms of the Whitney polynomial and the terms occurring in the subtraction process that we use to eliminate those cases in which one or more neighbouring points are coloured alike.

In order to derive a transfer operator for calculating (6) we (figure 2) consider the effect of adding point D' to the lattice. We may, but need not, add one or both of the lines $D\,D'$ and $C'\,D'$ to each of the subgraphs G. Therefore, we need a record of whether or not C' and D were previously connected by lines in the subgraph G. Later on we shall need similar information about D' and E and so on as we go round the lattice, adding a point to each column in turn. How do we specify the sets into which these 'outside' points are connected up by the lines in each G? We can describe a typical situation by a notation like $\phi = (A\,B)\,(C)\,(D\,F\,G)\,(E)$, which means that A and B are connected C and E are isolated, while D, F and G form a connected group or set.

Consider now the possibilities relating to the line DD' (figure 2). If we add this line to any graph G, the point D' will now be connected to just the same 'outside' points as was D by the lines in G, and to no others. The effect is to increase r_G by one. Now suppose that we omit the line DD'. Point D' will now be unconnected with any of the other 'outside' points and two cases arise. If D was connected to other 'outside' points, we must replace, e.g. (DFG) by $(D')(FG)$. If D was isolated, we simply replace (D) by (D'). We describe these three possibilities by the factor $(x+D_D+E_D)$, where D_D corresponds to selecting those graphs in which D was isolated while E_D corresponds to an operation like $(DFG)\rightarrow(D')(FG)$, that is to isolating D' if D was *not* previously isolated. Similarly, we can examine the effect of adding the line $C'D'$ or omitting it. If we omit it, the rank, nullity and the connectivity situation are all unchanged. If we add this line, there are two possibilities. Either C' and D' were already connected by lines in G, in which case the number of circuits is increased by one, or else C' and D' were not connected by lines in G, in which case the addition of this line will increase the rank by one. Thus we can describe the three possibilities by the factor $(1+yP_{C'D'}+xQ_{C'D'})$ where operator $P_{C'D'}$ selects graphs in which points C' and D' are joined, while the operator $Q_{C'D'}$ selects graphs in which C' and D' are *not* joined, and then joins them.

Thus, we have a pair of operators the product of which takes account, for each subgraph G, of the possible contributions to the Whitney polynomial $W(x,y)$ of adding, or omitting, the two extra lines incident on a point such as D' (figure 2) and, at the same time, these operators ensure that a proper record of the connectivity of the set of 'outside' points is maintained for all cases. Consider the simple case of a lattice with three points in each row. There are five possibilities: All three points are isolated which we describe by $[(A)(B)(C)]$. All three points are connected which we describe by $[(ABC)]$. Two points are connected, but the third is isolated, which we describe by $[(AB)(C)]$, $[(AC)(B)]$ or $[(A)(BC)]$. Plainly there is a 1–1 correspondence between the possible ways in which M points in a row can be 'connected up' and the partitions of these points into sets. The rows and columns of the transfer matrix will correspond with these possible partitions, and the matrix elements of the operators we have just been discussing are readily written down. For example:

$$\left.\begin{aligned} P_{AB}[(AB)(C)] &= [(AB)(C)],\\ Q_{AB}[(AB)(C)] &= 0,\\ P_{AB}[(A)(BC)] &= 0,\\ Q_{AB}[(A)(BC)] &= [(ABC)],\\ D_A[(AB)(C)] &= 0,\\ D_A[(A)(BC)] &= [(A)(BC)],\\ E_A[(AB)(C)] &= [(A)(B)(C)],\\ E_A[(A)(BC)] &= 0, \end{aligned}\right\} \tag{7}$$

correspond to the above definitions of the operators in words. In this representation the P's and D's are wholly diagonal, the E's and Q's are wholly non-diagonal.

We can now verify that the operators described above do take proper account both of the changes in connectivity of the 'outside' set of points and of the weights to be given to each possible subgraph in the Whitney polynomial as we build the lattice up one point at a time. The transfer matrix is thus a product of pairs of such operators. (We make the usual assumption that the lattice is wrapped round a cylinder, so that column M+1 is identical with column 1. For M large, it makes little difference whether we dispose our points on the cylinder in 'screw' fashion or in successive rings, and the difference can easily be investigated in a particular case.)

We impose a further boundary condition (standard in this type of problem) that the initial and final connectivities are to be the same after a large number of lattice points have been added, in other words that if we begin with the connectivity $(A)(B)(C)$ we restrict ourselves to graphs in which the last three points added are also isolated from one another, and similarly for other initial connectivities. This means that we must work with the *trace* of the transfer matrix. As usual, this corresponds simply to identifying the first row of points with the (N+1)th. Since the transfer matrix is effectively the N-th power of an operator corresponding to adding one row, and we are concerned with the case of large N, the problem is also that of finding the largest eigenvalue of the transfer operator for one row, which itself consists of a product of M pairs of operators of the type described above.

6. Abstract properties of the transfer operators

Certain results can be proved from the abstract properties of these operators without use of any representation of them. We have, for example,

$$P_{AB}^2 = P_{AB}, \quad Q_{AB}^2 = 0, \quad P_{AB}Q_{AB} = Q_{AB}, \quad Q_{AB}P_{AB} = 0$$

and analogous properties of the D's and E's. Also

$$D_A P_{AB} = P_{AB} D_A = 0, \quad D_A Q_{AB} = 0, \quad P_{AB} E_A = 0. \tag{8}$$

We notice from (7) that the P's and D's leave the number of parts of any partition the same, every Q reduces the number of parts by one, while every E increases the number of parts by one. Therefore, if any product of such operators is multiplied out, the only terms that can contribute to a trace are those which contain equal numbers of Q's and E's. It follows that the trace of any such operator is unaffected by the transformation

$$Q_{ij} \to \alpha Q_{ij} \quad E_i \to \alpha^{-1} E_i \tag{9}$$

(provided that α is independent of i and j and is a number not an operator). The interpretation of the terms in the transfer matrix that arise solely from products of the Q's and E's is immediate. Consider the product

$$\ldots(1+x_H Q_{BC})(x_V+E_B)(1+x_H Q_{AB})(x_V+E_A)\ldots. \tag{10}$$

We have made a distinction between horizontal and vertical lines of the lattices by giving them separate selector variables x_H and x_V but otherwise this operator is

obtained from the product of operators that generates the Whitney polynomial by omitting all the terms involving P's and D's. Which subgraphs does the trace of (10) enumerate?

If we start and finish with all M points in a row connected we enumerate just the trees on the lattice. The absence from (10) of all terms involving the P's means that the graphs involved cannot contain any circuits, while the fact that there are no terms involving D's means that we are concerned only with one-component graphs. (We give in the appendix the straightforward, but rather lengthy, graph-theoretical argument on which the last statement is based. For the plane square lattice, it follows also from the duality relations that we shall prove shortly.) Other matrix elements making up (10) correspond to our starting and finishing with graphs containing more than one component, that is to say with 'forests' of two or more non-overlapping trees. By using relations (8), the operators for the Whitney polynomial can be factorized, and instead of (10), we have, for the whole transfer operator

$$\ldots(1+x_H Q_{BC})(1+yP_{BC})(x_V+E_B)(1+D_B x_V)\ldots. \tag{11}$$

The trace of any product of the Q's and E's either vanishes, or designates a tree (together with the 'forest' generated from it by omitting one or more of the branches in the first and last rows of the lattice). The effect of the factors involving the P's and D's is to weight some of the trees with factors of the type 1, $1+y$ or $1+1/x_V$, the precise number of such factors depending on the particular tree and on the order in which the factors come in (11). Tutte (1954) showed that, if we take all the trees in the lattice and weight each one of them according to a rather complicated prescription based on putting all the lines in the lattice in some sort of dictionary order, looking at each tree and weighting each line in the lattice using, for each, one of these factors 1, $(1+y)$ or $(1+1/x)$, we arrive at what Tutte calls the 'dichromate' of the lattice, which, to a factor, is just the Whitney polynomial (6). It can, in actual cases, be explicitly verified that the process indicated by (11) is equivalent to numbering the lines of the lattice in a particular way and then applying Tutte's prescription (1954) (the result of which he proved to be independent of the numbering convention actually used).

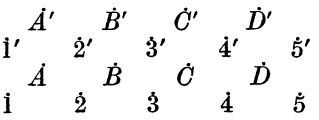

FIGURE 3

To derive the dual relations between these operators let figure 3 represent a small portion of the original lattice denoted by letters. As usual, the dual lattice is built up of points, one for each empty polygon, which are denoted by numbers. Corresponding lines, e.g. $1'2'$ and AA', or $22'$ and AB intersect at right angles. We associate graphs on the original lattice with graphs on the dual lattice according to the following rule. If a line, e.g. AA', is present in the original graph its counterpart

$1'\,2'$ is *absent* from the associated graph on the dual lattice and vice versa. In figure 3, we suppose that the dual lattice has been built up as far as the lines $1'\,2'$, $2'\,3'$, $3'\,4'$, etc., so that $1'$, $2'$, $3'$, etc. are 'outside' points and that the original lattice has been built up as far as the lines $A\,A'$, $B\,B'$, $C\,C'$, so that A', B', C' are 'outside' points in the original lattice. (Lines like $A'\,B'$, $B'\,C'$ have not yet been added.) In the dual lattice the operator $P_{2'3'}$ selects just those graphs for which the points $2'$, $3'$ are connected, either directly by the line $2'\,3'$, or else indirectly by paths like $2'\,2\,3\,3'$. The assertion that there is, in the dual lattice, such a direct or indirect path connecting $2'$ and $3'$ is equivalent to saying that, in the original lattice, there is *no* path connecting B' with either A' or C' nor, for that matter, with any of the other 'outside' points like D' in the original lattice. Furthermore any path connecting B' and C' on the original lattice (with the exception of the direct line $B'\,C'$ which has not yet been added to it) must inevitably cross somewhere any path that connects $2'$ and $3'$ on the dual lattice (since we may not use lines like $B'\,C'$).

In other words, if we associate graphs on the original lattice with graphs on the dual lattice by the rule just given, the operator $P_{2'3'}$, selecting graphs in which $2'$ and $3'$ are joined in the dual lattice, is equivalent to the operator $D_{B'}$, which selects graphs on the original lattice for which B' is isolated from all other 'outside' points. Reciprocally, we can infer the equivalence of $D_{3'}$ and $P_{B'C'}$, etc. We can also infer the equivalence of operators like $Q_{2'3'}$ and $E_{B'}$. For $Q_{2'3'}$ selects those graphs in which $2'$ and $3'$ are *not* connected in the dual lattice and then introduces such a connexion, and this is easily seen to be the counterpart of selecting those graphs in which B' is connected to at least one of the outside points $A', C', D', \ldots$, on the original lattice and then isolating B' from all of them.

It is easily verified that this dual relationship between operators has the relationship of Whitney (1932)

$$\mathrm{W_L}(x,y) = x^{rL}y^{nL}\,\mathrm{W_L}\left(\frac{1}{y},\frac{1}{x}\right) \tag{12}$$

as a particular consequence. Sykes & Essam's (1964) relations between the generating functions for the expected numbers of components of a graph and its dual then follows as a particular case, using (6*a*).

7. Particular representations of the transfer operators

A fairly obvious principle to try out is to represent the nodes of connexion among the points, $A, B, C \ldots$ as follows:

$$(A) \text{ by } \left(\frac{1+\mu_A}{2}\right), \quad (AB) \text{ by } \left(\frac{1+\mu_A\mu_B}{2}\right), \quad (ABC) \text{ by } \left(\frac{1+\mu_A\mu_B\mu_C}{2}\right), \text{etc.} \tag{13}$$

so that, for example the mode of connexion

$$(A)\,(BCD)\,(EF) \text{ is represented by } \left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B\mu_C\mu_D}{2}\right)\left(\frac{1+\mu_E\mu_F}{2}\right).$$

It is then easy to obtain related representations of particular combinations of the operators P and Q and of D and E. For example, it is readily verified that D_A+E_A is represented by $\frac{1}{2}(1+S_A)$ because this operator sends

$$\left(\frac{1+\mu_A}{2}\right)\to\left(\frac{1+\mu_A}{2}\right);\quad \left(\frac{1+\mu_A\mu_B\mu_C}{2}\right)\to\left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B\mu_C}{2}\right), \tag{14}$$

i.e. it sends $(A)(BC\ldots)$ into itself and (ABC) into $(A)(BC)$, etc. Moreover, $1+C_AC_B$ can represent $2P_{AB}+Q_{AB}$ because it sends

$$\left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B}{2}\right)\to\left(\frac{1+\mu_A\mu_B}{2}\right);\quad \left(\frac{1+\mu_A\mu_B\mu_C}{2}\right)\to 2\left(\frac{1+\mu_A\mu_B\mu_C}{2}\right). \tag{15}$$

However, these results proved difficult to generalize, the factors of 2 in (15) are very troublesome and a fundamental flaw in this representation was found. We have seen that for M = 3 there are five different possible modes of connexion but the above representations of them are *not*, as they should be, linearly independent. For M large, there are too few linearly independent functions of the μ's, 2^M in fact, to match the number of possible modes of connexion of a row of M points, which, as we shall see presently, is asymptotically proportional to 4^M for a planar lattice.

However, some of the results suggested by (14) and (15) are, in fact, correct. If these representatives were truly linearly independent, the problem of calculating the trace of the corresponding transfer matrix would become equivalent to the solution of the Onsager problem (1944) (after making the transformation of operators $C_r\to S_r$; $S_r\to C_r$). In fact Kasteleyn & Fortuin (1969) have shown, by an entirely different method, that the Onsager problem without magnetic field is, in fact, equivalent to the result suggested by (14) and (15), namely to an enumeration of the subgraphs of the lattice according to their numbers of lines, an extra factor of 2 being inserted for every independent circuit in each subgraph. (According to (15) a factor 2 is associated with each P type operator.)

The above suggests that we need 2M spin variables to form the basis of a representation of all the distinct ways in which M points $A, B, C, \ldots$ in an open row can be connected. We first classify those 'modes of connexion' that are possible on a *planar* lattice. (Already, for M = 4, we notice that the mode $(AC)(BD)$ is impossible, since it certainly implies some crossing of bonds. We are already aware of quite a number of enumeration problems that become impossible if the lattice is non-planar so we shall be wise to take account of this point.) Point A in the row is either isolated, or is connected to one or more other points in the row. Choose the farthest of these from A, say K, then K cannot be connected to any point to its right but may be connected to any or all of the points between it and A. Because of the existence of the connexion between A and K none of the points between A and K can be connected to points to the right of K without some crossing of bonds. Let $f(n)$ be the number of ways of connecting up n points in a row, subject to the above restriction. Then

$$f(n)=f(n-1)+f(n-2)+f(n-3)f(2)+f(n-4)f3)\ldots. \tag{16}$$
$$\text{mode}\,(A)\quad \text{mode}\,(AB)\quad \text{mode}\,(AC)\quad \text{mode}\,(AD)$$

The first term corresponds to point A being isolated. There are then $f(n-1)$ ways of connecting up the remaining points. If A is connected solely to B, there are $f(n-2)$ ways of connecting up the remaining $n-2$ points. If point A is known to be connected, at the farthest, to point C, point C may, or may not, be connected also to point B hence the factor $f(2)$. The factor $f(n-3)$ then describes possible modes of connexion of the $n-3$ points to the right of C. If point A is known to be connected, at the farthest, to point D, point D may, or may not, be also connected to either or both of points B and C, hence the factor $f(3)$ and the factor $f(n-4)$ describes the modes of connexion of $n-4$ points to the right of D, etc. Equations such as (16) occur in a large number of enumeration problems, and the generating function is of a well known type.

Defining

$$g(z) = \sum_{n=1}^{\infty} f(n)\, z^n,$$

we find easily from (16) that

$$g(z) = \frac{1-2z-(1-4z)^{\frac{1}{2}}}{2z}. \tag{17}$$

Equation (17) confirms the statement that the number of possible modes of connexion is ultimately proportional to 4^{M}.

We have already stated that a very large number of sets of objects of mathematical and physical interest are enumerated by (17). For example:

The quantum states of an assembly of 2M electrons, with total spin zero (which implies a magnetic moment of zero).

The number of independent commutators that can be formed of M + 1 operators.

The number of 'lattice permutations' (in the mathematical sense) of 2M numbers in an (M × 2) Young tableau.

The number of even–odd pairings of 2M points round a circle that can be realized without any crossing of the straight lines joining the M pairs.

The number of one-dimensional random walks of 2M steps, each of which may be to the right or the left, that eventually return to the origin, subject to the condition that no part of the walk ever goes to the left of the origin.

We follow the treatment of the Heisenberg problem used by Húlthen (1938) and others. We study an assembly of 2M spins which we label by numbers and use the bracket notation [1 2] to mean $(\mu_1-\mu_2)$, etc. We can show inductively that there is a (1–1) correspondence between their wavefunctions with total spin zero and the possible modes of connexion of an 'outside' row of M points on a planar lattice. Using the classification (16), we begin with [1 2] whenever the first 'outside' point A in the lattice is isolated, we begin with [1 4] whenever the mode of connexion on the lattice is of type $(A\,B)$, with [1 6] whenever the mode of connexion is of type $(A\,C)$, with [1 8] whenever it is of type $(A\,D)$, etc. Proceeding inductively, we can infer from equation (16) a 1–1 correspondence between Húlthen type wavefunctions involving 2M spins and possible modes of connexion involving a row of M points on

a planar lattice given that it exists for smaller values of M. Specifically, we have for

$$\mathrm{M}=2 \quad [1\,2][3\,4]\rightarrow(A)(B),[1\,4][2,3]\rightarrow(A\,B),$$

and for

$$\left.\begin{aligned}\mathrm{M}=3 \quad & [1\,2][3\,4][5\,6]\rightarrow(A)(B)(C),\\ & [1\,2][3\,6][4\,5]\rightarrow(A)(B\,C),\\ & [1\,4][2\,3][5\,6]\rightarrow(A\,B)(C),\\ & [1\,6][2\,3][4\,5]\rightarrow(A\,B\,C),\\ & [1\,6][2\,5][3\,4]\rightarrow(A\,C)(B).\end{aligned}\right\} \tag{18}$$

Húltheu (1938) studied the problem of a one-dimensional array of electrons with a nearest-neighbour interaction of Heisenberg type, with $\Delta = 1$ in (1). Such an 'isotropic' Heisenberg interaction can be reduced to a permutation operator $1-\mathrm{T}_{12}$ where T_{12} sends μ_1 and μ_2 into one another. We have, in fact

$$\left.\begin{aligned}(1-\mathrm{T}_{12})[1\,2] &= 2[1\,2],\\ (1-\mathrm{T}_{23})[1\,2][3\,4] &= [4\,1][2\,3],\\ (1-\mathrm{T}_{23})[4\,1][2\,3] &= 2[4\,1][2\,3].\end{aligned}\right\} \tag{19}$$

That is to say that these permutation operators are of just the type we require for discussing connexion problems on a lattice. $(1-\mathrm{T}_{12})$ always has [1 2] as end-result, corresponding, according to (18), to configurations with point A isolated and must therefore represent $2D_A+E_A$. Also, according to (19), $(1-\mathrm{T}_{23})$ will always have [2 3] as end result. Examination of representation (18) shows that [2 3] always means that points A and B on the lattice are connected (and analogous results are true generally) and we conclude that operator $(1-\mathrm{T}_{23})$ represents $2P_{AB}+Q_{AB}$.

Thus, we are saddled with unwanted factors of two of the same type as that which appeared in (15). However, we have got over the fundamental difficulty that vitiated representations of the type (13), since we can now prove formally that the number of independent Húlthen wavefunctions for 2M spins is precisely the same as the number of *admissible* modes of connecting up M points in a row on a planar lattice. (An inductive argument, based on a comparison of expressions (16) and (18), in fact shows how to set up a (1–1) correspondence between these two sets of entities.) We are led to look for transformations of these operators which nevertheless retain the form of the relations (19), but with different numerical coefficients. Such transformations indeed exist, but the transformed operators are complicated.

The most useful type of operator to replace $(1-\mathrm{T}_{12})$ in (19) seems to be the following:

$$U_{12}=\left[\frac{r}{s}+C_1C_2\right]\frac{(1+s_1)(1-s_2)}{4}+\left[\frac{s}{r}+C_1C_2\right]\frac{(1-s_1)(1+s_2)}{4}, \tag{20}$$

which was found by a systematic study of operators obeying relations like (19). The Húlthen type wavefunction is replaced by

$$[1\,2]=r\,\frac{(1+\mu_1)(1-\mu_2)}{4}+s\,\frac{(1-\mu_1)(1+\mu_2)}{4}, \tag{20'}$$

which reduces to $\mu_1 - \mu_2$ if $r = -s = 2$ for which case (20) reduces to $(T_{12} - 1)$ and we recover (19). Using these new operators and Húlthen symbols it will be found that, instead of relations (19) we have, for example,

$$\left.\begin{aligned} U_{34}[3\,4] &= \left(\frac{r}{s}+\frac{s}{r}\right)[3\,4], \\ U_{34}[2\,3][4\,5] &= [2\,5][3\,4], \\ U_{34}[3\,6][4\,5] &= [3\,4][5\,6], \\ U_{34}[1\,4][2\,3] &= [1\,2][3\,4]. \end{aligned}\right\} \tag{19'}$$

In these relations, we suppose that the 2M electrons are arranged in a ring and are numbered in a line $1, 2, 3, \ldots, n-1, n$. The last three relationships can be represented graphically. They correspond to the three situations that can occur if 3 and 4 are in different brackets. The two points joined to 3 and 4 can be both to the left of 3, both to the right of 4, or 3 can be joined to a point on its left and 4 to a point on its right. These situations are shown graphically in figure 4.

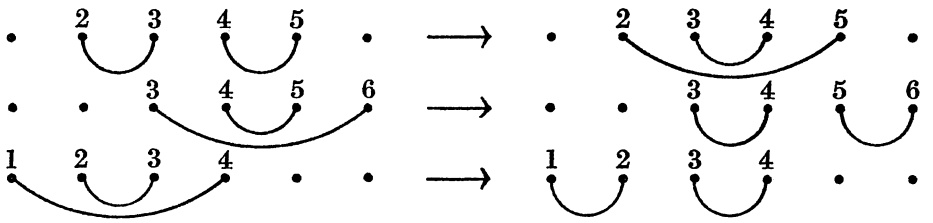

FIGURE 4

This represents the three topologically distinct ways in which electrons 3 and 4 can each be associated with one other electron, without any crossing of lines, that is, excluding functions like [1 4][2 5]. It is known that sets of wavefunctions such as (18), in which each bracket contains one odd and one even number and 'crossings' are not allowed, form a linearly independent set. In the appendix, we prove that the more general functions formed out of 'generalized Húlthen brackets' like (20') are also linearly independent. Relations (19') differ slightly in form from (19) in that in (19') two numbers in a bracket always appear in their natural cyclic order.

We now suppose that these electron spins are disposed on the *lines* of an auxiliary lattice, which is related to the points on the original lattice (shown in brackets as $(A)(B)(C)$, etc.) in the manner shown in figure 5. This exhibits a relationship between a row of M points in the original lattice and a set of 2M lines that we group into odd–even pairs, according to Húlthen's formalism. As exemplified in expressions (18), each possible way of grouping the lines into odd–even pairs is associated with a mode of 'connecting up' a row of M points on the original lattice by bonds in this lattice. Thus, the presence of [1 2] means that point (A) is isolated, the presence of [2 3] means that points (A) and (B) are joined, etc. It can be verified that

operators (20) represent the following abstract operators (see the definitions of P_{AB}, Q_{AB}, D_A, E_A in § 5).

$$U_{12} = \left(\frac{r}{s}+\frac{s}{r}\right) D_A + E_A; \quad U_{23} = \left(\frac{r}{s}+\frac{s}{r}\right) P_{AB} + Q_{AB}.$$

The μ's in (20) and (20′) are associated with the *lines* of the auxiliary lattice shown in figure 5.

We shall be interested in finding the trace of a product such as

$$\ldots(1+xU_{45})(1+xU_{23})\ldots(1+XU_{34})(1+XU_{12})\ldots, \tag{21}$$

where the selector variables x and X are usually different for a problem of 'percolation' or 'chromatic' type. Also in the 'percolation' problem we are interested in the case $r/s+s/r = 1$, i.e. r/s is complex. We shall show presently that, apart from these analytic complications, the finding of the trace of an operator such as (21) is effectively equivalent to solving problems of 'generalized ice' type as effected by Lieb (1967*a* to *d*).

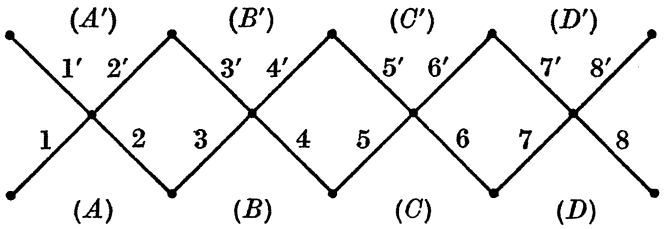

FIGURE 5

Both the mathematical treatment and the interpretation of 'ice-like' problems are very much simplified if we build up our lattice diagonally instead of horizontally or vertically. Lieb (1967*a* to *d*) solved his problems by setting up operator relations between 'arrow configurations' in successive rows of vertical arrows (thus losing the symmetry between vertical and horizontal). Their operator structure is complicated, and their relationships with Heisenberg type problems only become apparent when their eigenfunctions are found. From the new point of view, the relevant Heisenberg-like operators can be written down almost directly, for an 'ice-type' problem or for the problem on the auxiliary lattice that we associate with a 'percolation type problem'.

We use a new method of building up a plane square lattice, line by line this time. We associate a 'spin' variable with each line, according to the direction of its arrow, and we number the lines according to the conventions shown in figures 5 and 6*a*. We turn the plane square lattice anticlockwise through 45° (compare figure 6*b*). Each row of lines is built up, one line at a time, and the lines are added in the order 1 2 3 ... 1′ 2′ 3′ ... 1″ 2″ 3″ (figure 6*a*). These remarks apply both to the actual lattice in an 'ice-like' problem or to the auxiliary lattice that we use in a 'percolation' type problem. An arrow (or spin variable) is associated with each of the lines in figure 6*a* or 6*b*.

We restrict ourselves again to arrangements of arrows such that, at each node of the lattice shown in figure 5 there are 0, 2 or 4 arrows in the positive directions. We use the convention that a positive direction of arrow is upwards or to the right (figure 6*b*) and is associated with $\mu = +1$, or with $\frac{1}{2}(1+\mu)$. The result of this restriction is that there are again eight possible types of node (figure 7). If we wish to assign different weights to them, we can do this by means of operators of generalized

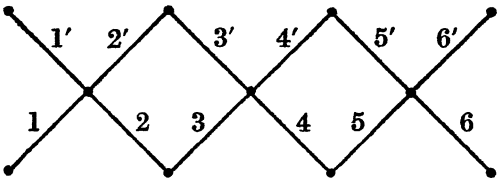

FIGURE 6*a*

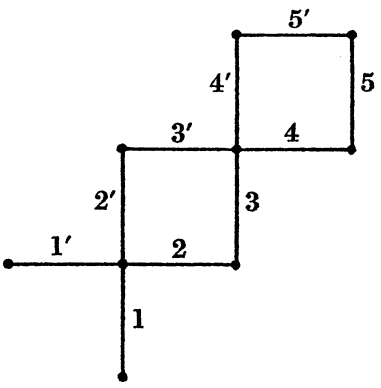

FIGURE 6*b*

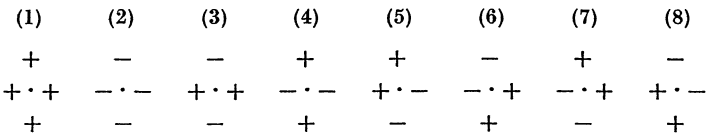

FIGURE 7

Heisenberg type. Suppose that we have added all the lines forming the row (1 2 3 4 5 ...) in figure 6*a*. The operator describing the possible ways of adding the pair of lines 1′ 2′ can now be written down as a sum of terms, one term corresponding to each permitted type of node. The conventions for distinguishing node types are exhibited in figure 7 in terms of positive and negative signs and will be found to agree with those of figure 1 (which are expressed in terms of arrows).

The form of operator that we now use is associated with a sum of terms, one corresponding to each of these types of node. The operator associated with the node of type (4) is, for example, $C_1C_2(1+S_1)(1-S_2)/4$. In words, we first select from all the possible configurations of the row (1 2 3 4 ...) (figure 6*a*) those corresponding to bond 1 being positive and bond 2 negative, by means of the operator $\frac{1}{4}(1+S_1)(1-S_2)$. The further operator C_1C_2 now changes $\frac{1}{4}(1+\mu_1)(1-\mu_2)$ to $\frac{1}{4}(1-\mu_1')(1+\mu_2')$ in view of the fact that this correctly describes the configuration (1′ negative, 2′ positive) of the two remaining bonds at a node of type (4) (see figures 6*b* and 7). For some types

of node the operator C_1C_2 is absent, for example the operator corresponding to the addition of a node of type (1) is just $\frac{1}{4}(1+S_1)(1+S_2)$ (see figure 7). The effect of restricting ourselves to nodes with even numbers of positive arrows is that operators C_1 and C_2 never appear separately.

Rather than writing down these 'Heisenberg-like' forms of each of the operators corresponding to nodes of types (1) to (8), it is more illuminating to define each of the operators J_1 to J_8 as the effect of adding the corresponding type of node to the lattice in the position (1 2, 1′ 2′) and to express operators such as C_1C_2, S_1S_2, etc. in terms of them.

TABLE 1

$$
\begin{aligned}
I &= J_1+J_2+J_7+J_8\\
S_1S_2 &= J_1+J_2-J_7-J_8\\
S_1 &= J_1-J_2+J_7-J_8\\
S_2 &= J_1-J_2-J_7+J_8\\
C_1C_2 &= J_3+J_4+J_5+J_6\\
C_1C_2S_1S_2 &= -J_3-J_4+J_5+J_6\\
C_1C_2S_1 &= -J_3+J_4+J_5-J_6\\
C_1C_2S_2 &= -J_3-J_4+J_5-J_6
\end{aligned}
$$

For the first four 'diagonal' operators the configurations of the 'initial' pair of bonds (1 2) and the 'final' pair of bonds (1′ 2′) are the same, for the last four 'off-diagonal' operators the signs of bonds 1 and 2 are both reversed.

In the original 'ice' problem we excluded nodes of types 7 and 8 because (see figure 1) they correspond to all arrows pointing respectively away from the node or towards it, which are excluded by the 'ice' condition. All the other types of node from 1 to 6 are permissible and are weighted equally. Therefore, the problem of calculating the entropy of the 'ice' model reduces to that of calculating the trace of the product of operators of the type $[\frac{1}{2}(1+S_1S_2)+C_1C_2]$, one such operator for each node of the lattice. Similarly, for the generalizations of the 'ice' problem studied by Lieb (1967*a* to *d*), the relevant operators are now *weighted* sums of the operators J_1 to J_6, the relative weights given to them being the various Boltzmann factors appropriate to each type of node.

Obviously, the operator forms of these problems are greatly changed by this device of building up the lattice in a diagonal, rather than in a horizontal or vertical direction, and should lead to simpler treatments. We have shown that problems of the 'colouring' or 'percolation' type are also reducible to these 'generalized Heisenberg' problems. We have, however, the additional complication that the addition of one row of nodes 1 to M to the original lattice corresponds to the addition of a row of 2M lines to the auxiliary or 'Heisenberg' lattice shown in figures 5 and 6 and we have further pointed out that such problems will, in general, involve different selector variables for operators of the two types, U_{12}, U_{34}, U_{56}, etc., and U_{23}, U_{45}, U_{67}, etc.

It has been pointed out by Fan & Wu (1970) that symmetry and other relations lead to a very large number of possibilities of transforming these 'ice-like' problems into one another. The device of building up the lattice diagonally rather than horizontally or vertically obviously opens up a whole fresh set of such possibilities.

8. The general Whitney problem in operator form

We set out below the Whitney problem for a plane square lattice, express it in operator form and then convert it into a Heisenberg-like problem on the auxiliary plane square lattice. The problem will then be specialized to the 'percolation' and 'chromatic polynomial' cases.

The full Whitney problem is to evaluate the sum (over all subgraphs G of the lattice containing L points)

$$\sum_G = Z^{C_G} Y^{S_G} x_H^{l_H} x_V^{l_V} \mathrm{W}(x_H, x_V, Z, Y), \tag{22}$$

where $(\mathrm{L} - C_G)$ and S_G are respectively the rank and nullity of G, and l_H, l_V are the numbers of horizontal and vertical bonds in G. Z, Y, x_H, x_V are the corresponding selector variables. Because of the Euler relation.

$$C_G = \mathrm{L} - l_H - l_V + S_G$$

one of these four selector variables is redundant. (We have three independent selector variables compared with Whitney's two because we desire to keep separate records of the vertical and horizontal bonds in G.)

In operator form the evaluation of W is equivalent to finding the trace of the product of the following type

$$\mathrm{W}(x_H, x_V, Z, Y) = \mathrm{tr}\,\Pi\,(x_V + ZD_A + [E_A/\alpha])\,\Pi\,(1 + Yx_H P_{AB} + \alpha x_H Q_{AB}), \tag{23}$$

one factor for each horizontal or vertical bond on the lattice, where, as we have seen from equation (9), α is a parameter that can be chosen arbitrarily without affecting the trace. We can write this relationship slightly more symmetrically thus

$$x_V^{-\mathrm{L}}\,\mathrm{W} = \mathrm{tr}\,\Pi \ldots \left(1 + \frac{Z}{x_V} D_A + \frac{E_A}{\alpha x_V}\right) \Pi\,(1 + Yx_H P_{AB} + \alpha x_H Q_{AB}) \ldots, \tag{24}$$

and the dual transformation can be shown, by applying the argument that led to equation (12), to send

$$x_H^{-1} \to x_V', \quad x_V^{-1} \to x_H', \quad Y^{-1} \to Z', \quad Z^{-1} \to Y', \tag{25}$$

i.e. the dual transformation interchanges horizontal and vertical lines present and absent and also components and independent circuits present and absent. Equation (12) is a particular case of this.

For the theory given above to be applicable, the ratio of the coefficients of D_A and E_A must be the same as the ratio of the coefficients of P_{AB} and Q_{AB}, which implies $\alpha^2 = YZ$. If, in expression (20), we write e^θ for r/s and use (19) we conclude that

$$U_{12} \quad \text{represents} \quad 2\cosh\theta D_A + E_A,$$

$$U_{23} \quad \text{represents} \quad 2\cosh\theta P_{AB} + Q_{AB}.$$

With the above choice of α, the selector variables appearing in expression (20), that is in the operator product

$$\ldots(1 + XU_{12})\,(1 + XU_{34}) \ldots (1 + xU_{23})\,(1 + xU_{45}) \ldots \tag{26}$$

are related to the selector variables occurring in the Whitney polynomial (22) as follows

$$X = Z^{\frac{1}{2}}/Y^{\frac{1}{2}}x_V, \quad x = Y^{\frac{1}{2}}x_H/Z^{\frac{1}{2}}, \quad 2\cosh\theta = (YZ)^{\frac{1}{2}}. \tag{27}$$

The chromatic polynomial is, to a factor, the Whitney polynomial for the following special values of these variables: $Z = 1$, $Yx_H = -1$ (a weight of -1 for each line completing a circuit), $x_H = x_V = -1/k$ (a weight of $-1/k$ for each other line) from which we conclude that in (26) $X = -k^{-\frac{1}{2}}$, $Y = k$, $x = -k^{\frac{1}{2}}$, $2\cosh\theta = k^{\frac{1}{2}}$. In terms of the J operators, Table 1 and expression (20) of text, we have

$$U_{12} = J_3 + J_4 + \mathrm{e}^{-\theta}J_7 + \mathrm{e}^{\theta}J_8.$$

For the particular choice of selector variable occurring in the chromatic polynomial the weights given to each type of node by the operator $1 + XU_{12}$ are indicated by

$$1 + XU_{12} = J_1 + J_2 - k^{\frac{1}{2}}J_3 - k^{\frac{1}{2}}J_4 + (1 - k^{\frac{1}{2}}\mathrm{e}^{-\theta})J_7 + (1 - k^{\frac{1}{2}}\mathrm{e}^{\theta})J_8, \tag{28}$$

$1 + xU_{23}$ having an analogous expansion with $k^{\frac{1}{2}}$ replaced by $k^{-\frac{1}{2}}$. [The operators $J_1 \ldots J_8$ are of course different in the two cases operating respectively on $(\mu_1; \mu_2)$ and on $(\mu_2; \mu_3)$.]

We can also formulate the percolation problem as a particular case of the general Whitney problem expressed in operator form in (23) and (26). We are interested mainly in the expected number of disconnected components on the lattice as a function of x_H and x_V. This is given by

$$\bar{C}_G = \left[Z \frac{\partial}{\partial Z} \{\ln \mathrm{W}(x_H, x_V, Z, Y)\} \right]_{Y=Z=1}, \tag{29}$$

or we can calculate the sum of the expected numbers of components and circuits as follows

$$\bar{C}_G + \bar{S}_G = \left[Z \frac{\partial}{\partial Z} \{\ln W(x_H, x_V, Z, Z)\} \right]_{Z=1}, \tag{30}$$

where W is given by (23). The calculation of W itself is trivial for the special case $Y = Z = 1$, for we have simply that any of the L horizontal lines may be present or absent, so may any of the L vertical lines, and the generating function for all the subgraphs is simply

$$\mathrm{W}(x_H, x_V, 1, 1) = (1 + x_H)^{\mathrm{L}}(1 + x_V)^{\mathrm{L}},$$

since $Y = Z = 1$ weights all the subgraphs equally. The percolation problem is equivalent to calculating the differential coefficient with respect to Z, *afterwards* putting Z equal to 1. A more general version of the problem is to calculate W as a function of x_H, x_V and Z.

According to (24) this is the problem of calculating

$$x_V^{-\mathrm{L}}\mathrm{W}(x_H, x_V, Z, Z) = \mathrm{tr}\,\Pi\left(1 + \frac{Z}{x_V}D_l + \frac{1}{x_V}E_l\right) \times \Pi\,(1 + Zx_H P_{lm} + x_H Q_{lm}), \tag{31}$$

where we have put the disposable constant α equal to unity.

At present, we can give an exact solution of this problem in only one set of cases, that in which $x_H = 1/x_V = x$ (say). These are known (Sykes & Essam 1964, 1966), to be the critical cases of the percolation problem, for we have p_H, the probability that any given horizontal line is present is $p_H = x_H/(1+x_H)$ with a similar relation for p_V. Thus, for these cases $x_H x_V = 1$ implies $p_H + p_V = 1$, and $p_H + p_V \geqslant 1$ is the critical condition for large connected domains to form.

To evaluate $\mathrm{W}(x, 1/x, Z, Z)$ in the form (24) we want to calculate

$$\mathrm{tr}\,\Pi\,(1+xZP_{lm}+xQ_{lm})\ldots\,\Pi\,(1+xZD_l+xE_l)\ldots.$$

Using the representation (20) we conclude that this is equivalent to calculating

$$\mathrm{tr}\,\Pi\,(1+xU_{23})\ldots\,\Pi\,(1+xU_{12})\ldots, \tag{32}$$

where U_{12} represents $2\cosh\theta D_A + E_A$ and U_{23} represents $2\cosh\theta P_{AB} + Q_{AB}$ as before. For this problem

$$Z = 2\cosh\theta. \tag{33}$$

In terms of the J operators (table 1) we have

$$U_{12} = J_3 + J_4 + e^{-\theta}J_7 + \mathrm{e}^{\theta}J_8$$

with a similar expression for U_{23}. Also using table 1, we see that the operator $1+xU_{12}$ is represented by

$$1+xU_{12} = J_1 + J_2 + xJ_3 + xJ_4 + (1+x\,\mathrm{e}^{-\theta})J_7 + (1+x\,\mathrm{e}^{\theta})J_8, \tag{34}$$

and we suppose that the auxiliary lattice shown in figure 4 to be built up diagonally in the way shown in figure 5*a* and described above in words (p. 266). The addition of the lines $(1', 2')$ in figure 5*a* corresponds to the application of the operator $1+xU_{12}$, the addition of the lines $(3', 4')$ to the application of the operator $1+xU_{34}$ and so on. Proceeding to the next row of lines, the addition of the pair $(2'', 3'')$ corresponds to applying $(1+xU_{23})$, the addition of the pair $(4'', 5'')$ corresponds to applying $(1+xU_{45})$ and so on. That is to say that the addition of two rows of lines to the auxiliary lattice corresponds precisely to the successive application of the two operator products $\Pi(1+xU_{12})$ and $\Pi(1+xU_{23})$, which, in turn, corresponds to the successive application of the two operator products in (32) that is, to the addition of a row of points, and some or all of the lines incident to them, to the original lattice.

In the special case we are considering, $1/x_V = x_H = x$, the operators $1+xU_{12}$ and $1+xU_{34}$ both assign the following weights to the various types of node in the auxiliary lattice:

TABLE 2

node type	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
weight	1	1	x	x	0	0	$1+x\mathrm{e}^{-\theta}$	$1+x\mathrm{e}^{\theta}$

these weights being the same for both sets of operators. By taking two further steps, we can reduce this to a problem whose solution is known. We revert for a moment from a description of the node types in terms of spin variables (figure 7) to a description in terms of arrows (figure 1). Of the permitted types of node type (8) corresponds to a 'sink' of arrows, type (7) to a 'source' of arrows, all others corresponding to the

specification 'two in and two out'. We can therefore infer that, at all events if we have a 'torus' or 'screw' type of boundary condition so that there are no 'raw edges' of the original or of the auxiliary lattices, the numbers of nodes of types (7) and (8) must be exactly equal. It will, therefore, make no difference to the eigenvalues and traces of our operators if we replace both the weights $(1+x\mathrm{e}^{-\theta})$ $(1+x\mathrm{e}^{\theta})$ by the square root of their product $(1+x^2+2x\cosh\theta)^{\frac{1}{2}}$. We now apply the transformation corresponding to reversal of all the horizontal arrows in figure 1 which sends $J_1 \leftrightarrow J_4$, $J_2 \leftrightarrow J_3$, $J_5 \leftrightarrow J_7$, $J_6 \leftrightarrow J_8$, and changes the weights from those given in table 2 to those given in table 3 below. These are compared with the weights assigned to a 'generalized ice' problem of which the solution has been given by Sutherland (1967).

TABLE 3

node type	(1)	(2)	(3)	(4)	(5) & (6)	(7) & (8)
weight in transformed problem	x	x	1	1	$(1+x^2+2x\cosh\theta)^{\frac{1}{2}}$	0
weight in Sutherland's problem	$\mathrm{e}^{\delta/2T}$	$\mathrm{e}^{\delta/2T}$	$\mathrm{e}^{-\delta/2T}$	$\mathrm{e}^{-\delta/2T}$	$\mathrm{e}^{\epsilon/T}$	0

Comparison of these makes it evident that the problems are equivalent, if we make the identifications

$$x = \mathrm{e}^{\delta/T}; \quad 1+x^2+2x\cosh\theta = \mathrm{e}^{2\epsilon/T}\,\mathrm{e}^{\delta/T} \tag{35}$$

and introduce a multiplying factor $x^{\frac{1}{2}}$ for each node in the auxiliary lattice.

It is only in the special case $x_H x_V = 1$ that we can, at present, reduce the percolation problem to an 'ice-type' problem whose solution is known. If x_H differs from $1/x_V$ we can still carry through the same steps but we arrive now at what might be called a 'staggered ice' problem. By this we mean that now the auxiliary lattice has to be divided into two interlacing sublattices, with two different sets of weights for the six node types on the two sublattices. (Reference to figure 6*a* shows that the two sublattices in fact correspond to successive rows of nodes of the auxiliary lattice if we follow the plan of building it up diagonally described above.) This 'staggered ice' type of problem is akin to the antiferromagnetic Onsager–Ising problem. It can be handled by a suitable modification of the Bethe–Hülthen ansatz method, but we reserve discussion of this for another paper. For the present, we confine ourselves to deriving some exact results for the percolation problem in the critical cases $x_H x_V = 1$. (It is very reasonable that the critical cases of the percolation problem should correspond to equal weightings of the nodes in the two sublattices that make up the auxiliary lattice. In the Onsager–Ising antiferromagnetic problem the two sublattices become indistinguishable at the critical temperature.)

9. Exact results for the critical case of the percolation problem

Sutherland's (1967) result is that the transfer-matrix problem specified in table 3 has the same eigenfunctions as a Heisenberg type Hamiltonian with anistropy parameter Δ, where $2\Delta = 2\cosh(\delta/T) - \mathrm{e}^{2\epsilon/T}$ which, using (35) and (33), gives

$$\Delta = -\cosh\theta = -\tfrac{1}{2}Z; \quad \mathrm{e}^{\delta/T} = x. \tag{36}$$

In using the result given by Sutherland (1967) to evaluate the Whitney polynomial $W(x, 1/x, Z, Z)$ for the limiting case of a large lattice, the following points must be remembered:

(*a*) The auxiliary lattice has twice as many nodes as the original lattice (see figure 5, where letters represent nodes of the original lattice and numbers lines of the auxiliary lattice).

(*b*) The initial factor $x^{\frac{1}{2}}$ for each node of the auxiliary lattice, to allow for the differences between the weighting of the nodes in Sutherland's problem and in the transformed form of our problem. (See the comparison in table 3.)

(*c*) The version of Sutherland's problem which is of interest to us corresponds to an 'ice' type problem with electric field zero. For this, the relevant value of Sutherland's parameter, y, corresponding to the largest eigenvalue of our problem, is zero.

We can now use table 3 and relations (36) to transcribe Sutherland's result to our notation. We find, using (31), (32) and (34):

$$W(x, 1/x, Z, Z) = x^{\frac{1}{2}L} \exp\left[L \int \rho(k)\, dk \ln\left\{\frac{(Z+x)^2 + 1 + 2(Z+x)\cos k}{x + 1/x - 2\cos k}\right\}\right], \quad (37)$$

where $\rho(k)$ is a function related to Δ, that is to say to Z in this problem, by an integral equation (Yang & Yang (1966), equation (6*a*)). For the case $y = 0$ that we are interested in, this integral equation can be solved explicitly by changing the variable from k to α by the transformation

$$e^{ik} = \frac{e^{i\mu} - e^{\alpha}}{e^{\alpha + i\mu} - 1}, \quad (38)$$

where $\cos\mu = -\Delta = \frac{1}{2}Z$. In terms of this new variable, the Yang & Yang integral equation is soluble by Fourier transforms, and we find

$$\rho(k)\, dk = \frac{d\alpha}{4\mu} \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right), \quad (39)$$

which is valid for the interesting range of values $-1 < \Delta < 1$ (i.e. Z between 2 and -2). Using (38) and (39) in (37) together with the fact that the integral of $\rho(k)$ is $\frac{1}{2}$ (in conformity with the fact that for $y = 0$ there are just $\frac{1}{2}L$ factors in Sutherland's product expression for the largest eigenvalue of the transfer matrix), we find finally

$$W(x, 1/x, Z, Z) = x^{L} \exp\left[\frac{L}{4\mu}\int_{-\infty}^{\infty} d\alpha \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right) \times \ln\left\{\frac{(1 + 2x\cos\mu + x^2)\cosh\alpha - \cos 3\mu - 2x\cos 2\mu - x^2\cos\mu}{(1 + 2x\cos\mu + x^2)\cosh\alpha - (x^2+1)\cos\mu - 2x}\right\}\right], \quad (40)$$

where $\cos\mu = \frac{1}{2}Z = \cosh\theta$.

It is straightforward, but tedious, to verify that, in the special case $Z = 1$, this reduces to the required form $(1+x)^{2L}/x^{L}$. [By the substitution $s = \sinh(\frac{1}{2}\alpha)$ (40) reduces to straightforward contour integrations for this special value of μ.]

For the special case $x = 1$, that is to say with horizontal and vertical bonds each open with a probability $\frac{1}{2}$, the critical value in the symmetric case, (40) simplifies to the following generating function:

$$W(1, 1, Z, Z) = \exp\left[\frac{L}{4\mu}\int_{-\infty}^{+\infty} d\alpha \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right) \ln\left(\frac{\cosh\alpha - \cos 2\mu}{\cosh\alpha - 1}\right)\right]. \tag{41}$$

This integral has not yet been evaluated in closed form but its analytic behaviour is known, since it has already appeared in the exact treatment of Rys's F-model of an antiferroelectric (Lieb 1967*b*).

10. Discussion of the properties of generating function (41)

The integral can, in principle, be evaluated whenever μ is a rational multiple of π. The exact values in table 4 are enough to give a general idea of the behaviour of $\ln W$ as a function of μ or Z.

Table 4

μ	Z	$(1/L)\ln W$	
0	2	$4\ln[\Gamma(\frac{1}{4})/2\Gamma(\frac{3}{4})]$	$= 1.56632\ldots$
$\frac{1}{3}\pi$	1	$\ln 4$	$= 1.38629\ldots$
$\frac{1}{2}\pi$	0	$(4/\pi) \times$ Catalan's constant	$= 1.16624\ldots$
$\frac{2}{3}\pi$	-1	$3\ln\frac{4}{3}$	$= 0.86304\ldots$
π	-2	0	

Professor Cooper's results are given in the appendix (table 6). The case $Z = 1$, for which the generating function is trivial, is discussed above. The case $Z = 0$ is the problem of the number of trees on a plane square lattice, and checks with the value obtained from Kirchhoff's determinant (Temperley 1958). For $Z = -1$, table 3 shows that we recover the ice problem, all nodes being weighted equally for $x = 1$.

We infer that the form of $\ln W$ as a function of Z has a radius of convergence of 2. At $Z = 2$ the function has a natural boundary but all derivatives with respect to μ are finite (Lieb 1967*b*). At $Z = -2$, the generating function becomes oscillating, the contributions from even and odd values of $C_G + S_G$ cancelling out.

As already stated, (41), considered as a function of Z, is the generating function for $C_G + S_G$. At critical conditions the expected number of bonds is just L (2L bonds present each with probability $\frac{1}{2}$), so the expected numbers of circuits and components are equal. The integral is awkward to handle numerically, because of the logarithmic singularity at $\alpha = 0$. Professor D. C. Cooper has kindly tabulated the integral for us and estimated the first two derivatives with respect to $\ln Z$ at $Z = 1$, which gives the expected values of $C_G + S_G$ and $(C_G + S_G)^2$ for the percolation problem in the critical case. Unfortunately, the only comparison that is possible at present with series expansion work is with the two types of expansion, 'perimeter' and 'irreducible diagram' given by Sykes & Essam (1964, 1966). The convergence of either type of series *at* the critical probability $\frac{1}{2}$ is a matter for speculation, however, M. F. Sykes & J. W. Essam give (private communication) the following estimate for $\bar{C}_G$ on the

basis of much longer expansions now available. This is compared with the value obtained from (41) (table 5). Agreement can be considered excellent. Information is also available on mean sizes of components, but it is not easy to see how to make a valid comparison with (41), since (41) includes the contribution from isolated points in the subgraph, each isolated point contributing 1 to $\overline{C}_G$.

TABLE 5

Estimates of $\overline{C}_G$, the *expected* number of components for $p = \frac{1}{2}$	
from Professor Cooper's estimate of the derivative of (41)	$\overline{C}_G = \mathrm{L} \times 0.0980_7$
from eleven terms of perimeter series	$\overline{C}_G > \mathrm{L} \times 0.0939_7$
estimated contribution of remaining terms (from extrapolation)	$\mathrm{L} \times 0.004_1$

11. PROSPECT OF FURTHER ANALYTIC TREATMENTS OF INTERESTING PROBLEMS

We still have available only two *basic* analytic methods mentioned above, the Bethe–Húlthen 'ansatz' method and the Kaufman–Onsager 'spinor' method. The Bethe–Húlthen method depends for its success on fulfilment of the 'ice' condition or something equivalent, because, as we build up a lattice row by row, we must be able to assert that the total numbers of up and down spins remain constant from row to row. We have shown that a particular case of the percolation problem can be reduced to a problem of this type. Thus some versions of the Whitney polynomial problem can definitely be solved now for certain ranges of the selector variables. To what extent these ranges can be extended by analytic continuation and transformations of the problem still remains to be seen.

The situation of the Kaufman–Onsager (1949) method is rather different. We might expect to be able to factorize operators such as (20) (into the required form of products of exponentials of quadratic spinors) in special cases only. (We recall that the Onsager (1944) problem has itself only been solved for zero applied magnetic field.) Thus, if we use transformations like (19), we might expect to factorize an operator like (20) only if there were some definite relation between the selector variables, e.g. those for numbers of lines and numbers of circuits. If we consider the percolation operator (34), it can only be so factorized in the limiting case $Z = 0$, which, as has been pointed out above, enumerates trees and forests on the lattice, an already solved problem.

Since the Kaufman–Onsager method does not depend on the 'ice' condition, it is to be expected that it will solve problems outside the scope of the 'ansatz' method. An algebraic criterion determining whether or not an operator of the type occurring in (20) (when U is some linear combination of operators J_1 to J_8) can be so factorized would be very valuable.

Although it does not lead to anything new, it is, from this new point of view, instructive to look at the Onsager model with first and second nearest neighbour interactions. This can also be reduced to a 'generalized Heisenberg' type of problem in the manner of Fan & Wu (1969). Let the spins be arranged on a plane square

lattice. Draw all the bonds on the dual lattice that separate positive and negative spins. These boundaries form closed domains, and 0, 2, or 4 lines therefore pass through every node. Thus we have a problem to which the formalism (21) can be applied. Identifying positive arrows with lines and letting $e^{\pm H_1}$, $e^{\pm H_2}$ be the Boltzmann factors for like/unlike pairs of first/second nearest neighbours, we assign the weights shown in figure 8 to the eight types of node on the dual lattice.

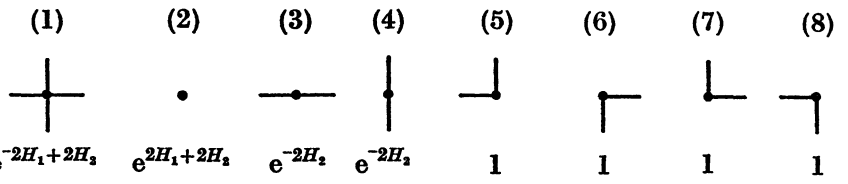

FIGURE 8

(The enumeration of pairs of first and second nearest neighbours is easily checked for each node.) The operator for each node on the dual lattice is easily written out, and it is readily verified that, for these weights, it can be factorized into

$$\tfrac{1}{2}(e^{2H_2}+1)\exp[-\tfrac{1}{2}H_1(S_1+S_2)][1+C_1C_2e^{-2H_2}]$$
$$\times[1+S_1S_2\tanh H_2]\exp[-\tfrac{1}{2}H_1(S_1+S_2)]. \quad (42)$$

The problem cannot be solved by the 'ansatz' method, because all eight types of node are involved. Although the operator *has* factorized, we cannot express *all* of S_1, S_2, C_1C_2, S_1S_2 in the required form as quadratic spinors! In the two limiting cases $H_1 = 0$ or $H_2 = 0$, we are concerned respectively with the smaller sets $C_1C_2, \ldots, S_1S_2$ or with $C_1C_2, \ldots, S_1, S_2, \ldots$, either of which *can* be so expressed. In either of these two cases we recover the Onsager (1944) problem.

It does not seem to be possible to derive the dimer problem *directly* as a limiting case of the Whitney polynomial. This contains terms of the type $Z^{\frac{1}{2}L}x_H^{l_H}x_V^{l_V}$ with $l_H + l_V = \frac{1}{2}L$, but many graphs of different structure also give rise to terms with the same powers of the selector variables. However Lieb (1967*e*), using a slightly different formalism, has shown that the dimer problem can be reduced to the estimation of traces of products of operators like $1+pC_1C_2(1+S_1)(1+S_2)$, which closely resembles the limiting form of (26) when the parameter α becomes large.

The problem of a mixture of monomers and dimers was formulated, though not solved, by Lieb (1967*e*), but only in terms of operators involving the C_r, by themselves, and thus not strictly of 'ice' type. The problem of 'rigid squares' in which a 'molecule' occupies a site on the lattice and the four neighbouring sites can also be formulated in this way, but again only in terms of operators involving odd powers of the C_r, and thus not of the 'ice' type.

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APPENDIX. PROOFS OF CERTAIN RESULTS ASSUMED IN THE TEXT

We prove the assertion made in the text that, if the operator product (23) is supposed to be expanded into individual products of operators of the type $\ldots D_A Q_{BC} E_C \ldots$ each such operator either vanishes or corresponds to just one possible subgraph on the lattice. Further, there is one D-type factor for every disconnected component of the subgraph. If we take any particular subgraph on the lattice, the rules given in the text tell us, at every step, which term to select out of the three that occur in every factor of the operator product (23). Furthermore, since the only operations described by this operator product are the addition or omission of bonds on the lattice, every term in this product must either vanish, if it calls for an impossible sequence of operations like P_{AB} followed by D_A, or else must correspond to a subgraph built up by such operations, that is to one of the subgraphs of the lattice.

Consider any disconnected component of a subgraph. In it we can define a unique point, which we call the summit, by the following rules:

(*a*) Take all the points that are connected, directly or indirectly by the lines in this component.

(*b*) Take the *highest row* of points in the lattice that has at least one point in set (*a*).

(*c*) Of the points in this row, take the one *furthest to the right* that is still in set (*a*).

This is the summit and there is exactly one summit for each component. Figure 9 represents a typical component of the subgraph. S is the summit of this component.

We claim that, if the operation of adding the point S' to the lattice is described by the operator D_S, then S, the point vertically below S', must be a summit. Consider the situation when the point S' has just been added. The operator D_S implies that: (*a*) S' is isolated after the addition of S' to the lattice *and* that (*b*) S was isolated immediately before S' was added (that is to say immediately after the addition of R'). Unless both these conditions are satisfied, the effect of D_S will produce an impossible operation, and the corresponding term would vanish in the operator product.

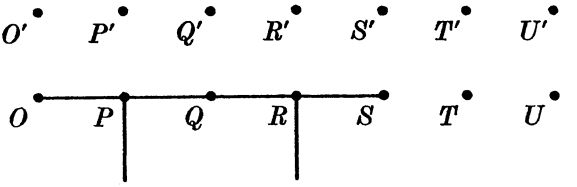

FIGURE 9

Now (*b*) implies that, immediately after the addition of R', S was not connected to R', Q', P' or O', that is S was not connected to any point to its left in the row immediately above it. Nor, since it was isolated, could S be connected to any point to its right, such as T or U in the same row. Further S cannot be connected to S', since the operator D_S in the operator product (23) implies the absence of the line SS', and the two points cannot be connected indirectly since by (*a*) and (*b*) they are both isolated from the set of points O', P', Q', R', T, U through which any such indirect path must pass. Since S is not connected to S', not to T nor to U, etc., it cannot be connected to any of the points T', U', etc., in the same row as and to the right of S' that are later added in the process of building up this row. This row therefore forms a barrier in the sense that no point in it can ever be connected to S. That is, we conclude that S is in the topmost row of the component. That it is the right-hand point follows easily. Suppose not. Then S is connected, via the bonds of the component, with some point, say U in the same row and to the right of S. It would be so connected at the moment of the addition of the point S' and the appropriate operation would then be E_S rather than D_S, because D_S only gives a possible operation if S is isolated. Thus we have a contradiction and can conclude that S *is* the right-hand point in the topmost row of the component.

Thus every summit point corresponds to a D operator. (A particular case of a summit is an isolated point with no lines incident to it.) There is exactly one summit point per component.

It is also necessary to prove linear independence for the 'wavefunctions' used in the text which consist of products of M 'generalized Húlthen brackets'. The generalized Húlthen bracket involves two of the spin-variables μ_i, μ_j.

$$[i,j] = \frac{r(1+\mu_i)(1-\mu_j)+s(1-\mu_i)(1+\mu_j)}{4}, \qquad \text{(A 1)}$$

where r and s are fixed constants. Our generalized 'wavefunctions' are products of M such brackets taken according to the following rules:

(a) In any bracket $i < j$.

(b) Every number between 1 and 2M appears just once.

(c) A pair of brackets $[a\,c][b\,d]$ with $a < b < c < d$ (which would correspond to 'crossing of bonds') never occurs.

We define 'round bracket symbols' $(i\,j)$ by the relation

$$(i\,j) = \frac{(1+\mu_i)(1-\mu_j)}{4} \tag{A 2}$$

and 'basic wave-functions' as products of M of these symbols not necessarily obeying the rules (a), (b), (c) but simply the conditions that there are exactly M positive spins and that each spin is mentioned once.

A generalized wavefunction is uniquely determined if we specify the first numbers in each of the M square brackets. Not all possible choices of these M numbers define possible wavefunctions, but two different generalized wavefunctions can never correspond to the same set of numbers.

Proof. Write the generalized wavefunction in the form

$$[a_1 b_1][a_2 b_2] \ldots [a_{\mathrm{M}} b_{\mathrm{M}}],$$

with $a_1 < a_2 < a_3 \ldots$. (Also $a_i < b_i$ because of (a) above.) Clearly $a_1 = 1$. We make some choice of the other $\mathrm{M}-1$ a's and try to choose the b's so that we have a permissible wavefunction. We must choose $b_{\mathrm{M}} = 1 + a_{\mathrm{M}}$. If we do not we must have a bracket $[a_j, 1+a_{\mathrm{M}}]$ with $a_j < a_{\mathrm{M}}$ and we cannot then choose any other number for b_{M} without violating (c). With the right-hand bracket fixed as $[a_{\mathrm{M}}, 1+a_{\mathrm{M}}]$, a repetition of the same argument shows that the only permissible choice of $b_{\mathrm{M}-1}$ is 'the smallest number above $a_{\mathrm{M}-1}$ that is not a_{M} or b_{M} that is, that has not already been used'. We proceed inductively, filling up the brackets in turn from the right, the choice at every step being determined by the rule: b_j is 'the smallest number greater than a_j that has not already been used'. It is easily shown inductively that rule (c) above is violated if any other choice is made for any of the b_j. On the other hand, it can happen at some stage that *no* b_j can be so chosen, which means that the corresponding choice of a_j's does not correspond to a permissible wave function. Thus, we can label any generalized wavefunction by specifying the particular choice of a_j's that gives rise to it. We can define a binary number by means of the a_j's, by replacing a_j by the power $2^{2\mathrm{M}-j}$. For example, for $\mathrm{M} = 3$, the permitted pairings are ordered in the following way:

$$\left.\begin{aligned}
&[1\,2][3\,4][5\,6] \to 2^5 + 2^3 + 2 = 42,\\
&[1\,2][3\,6][4\,5] \to 2^5 + 2^3 + 2^2 = 44,\\
&[1\,4][2\,3][5\,6] \to 2^5 + 2^4 + 2 = 50,\\
&[1\,6][2\,3][4\,5] \to 2^5 + 2^4 + 2^2 = 52,\\
&[1\,6][2\,5][3\,4] \to 2^5 + 2^4 + 2^3 = 56.
\end{aligned}\right\} \tag{A 3}$$

We call this binary number f and we can use it to label the generalized wavefunctions [square brackets]. We can also label the ϕ's (basic wavefunctions), by picking out

the M positive spins and introducing, as in (A 3), the term 2^{2M-j} whenever spin j is positive.

We now suppose the generalized wavefunctions to be expressed as linear combinations of the basic wavefunctions. Using (A 1) and (A 2) and remembering that the two types of wavefunction are obtained by multiplying the corresponding types of bracket together, we conclude, that if f is any binary number and ψ_f, ϕ_f are the corresponding generalized and basic wavefunctions that

$$\psi_f = r^M \phi_f + \text{other terms.} \tag{A 4}$$

The equality of the binary numbers specifying ψ_f and ϕ_f follows from (A 1) and the methods of constructing the ψ's and ϕ's. Inspection of (A 1) shows that the 'other terms' are obtained from ϕ_f by reversing the signs of the spins within one or more of the brackets in the product of round bracket symbols that make up ϕ_f. Since, for a permitted wavefunction ψ_f, a_j is less than b_j in any bracket, these interchanges will produce from ϕ_f other ϕ's described by a binary number larger than f. This means that the matrix relation between the ψ's and ϕ's is triangular, with the diagonal terms equal to r^M, any non-diagonal terms arising from ϕ's with a larger binary suffix than f.

The linear independence of the ϕ's is obvious. That of the ψ's now follows from (A 4), because, if f runs downwards in turn through the values that lead to a permissible ψ, at every stage we have at least one new ϕ (namely ϕ_f) which has never appeared in the previous equations. Further, it appears with the non-zero coefficient r^M. This proves linear independence, and in particular proves it for the particular case $r = -s$ corresponding to the Hülthen wavefunctions. We can now also infer completeness, because the number of spin-zero wavefunctions for 2M electrons is known to be

$$\frac{1}{M+1}\binom{2M}{M}$$

which also follows from generating function (17) of the text.

TABLE 6. VALUES OF (1/L) ln W CALCULATED BY COOPER FROM (41)

$Z = 2\cos\mu$	(1/L) ln W	$Z = 2\cos\mu$	(1/L) ln W
−2.0	0	0	1.16624_4
−1.8	0.41550_4	0.2	1.21480_9
−1.6	0.57220_7	0.4	1.26077_9
−1.4	0.68757_0	0.6	1.30450_4
−1.2	0.78191_7	0.8	1.34626_5
−1.0	0.86304_6	1.0	1.38629_4
−0.8	0.93492_3	1.2	1.42478_6
−0.6	0.99988_4	1.4	1.46190_6
−0.4	1.05944_3	1.6	1.49779_7
−0.2	1.11464_4	1.8	1.53258_3
0	1.16624_4	2.0	1.56632_0

At $Z = 1$, $\frac{1}{L}\frac{\partial(\ln W)}{\partial Z} = 0.196_2$. $\frac{1}{L}\frac{\partial^2 \ln W}{\partial Z^2} = -0.037_7$.

Analytic Properties of the Free Energy for the "Ice" Models

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The calculation of the free energy for the two-dimensional lattice models which obey the "ice" condition is reviewed and summarized. The analytic properties of this function relevant to thermodynamics are obtained for the set of those models corresponding to the absence of external fields. Detailed complex temperature Reimann structures are presented for the KDP and F models.

1. INTRODUCTION

The purpose of this paper is to analyze the thermodynamic properties of the planar "ice rule" ferroelectric models, which are isomorphic to a lattice statistical problem defined by the following rules:

1. On every edge of an $N \times M$ square lattice an arrow is placed, pointing in one of two possible directions;

2. The canonical partition sum is restricted to those configurations in which there are two, and only two, arrows pointing towards each and every vertex. Thus each vertex must be one of the six types shown in Fig. 1.

3. The partition sum of the associated ferroelectric is given by

$$z = \sum_{\substack{\text{allowed} \\ \text{config.}}} \Pi_j w_j^{n_j},$$

where n_j is the number of times vertex j occurs in a given configuration; this configuration has energy e_j and the associated canonical weight

$$w_j = e^{-\beta e_j},$$

where $\beta = 1/kT$, in the customary notation. The e_j are shown in Fig. 1.

This paper reports the investigation of the dependence of the ordered state and associated phase transition, where it exists, on the two parameters ϵ_1 and ϵ_2 defined below. The exponents are the same throughout each region and there is no nonphysical dependence of an accidental nature on (ϵ_1/ϵ_2).

We also discuss the Riemann surfaces for the energy in the complex temperature plane. The free energy is evaluated in terms of elementary functions in two special cases.

2. REVIEW OF THE BASIC THEORY

To complete the description of the model, adumbrated in the introduction, we shall impose periodic boundary conditions both vertically and horizontally, although the former is not essential. We shall refer to a row of vertical arrows simply as a row, which then has the possibility of being in 2^N states ϕ. Rather than specifying the states of the horizontal arrows between the rows, it is sufficient to define a transfer matrix $T(\phi, \phi') = \sum e^{-\beta E}(\beta = 1/kT)$, where the sum is over all allowed configurations of horizontal arrows consistent with the lower row being in state ϕ' and the next higher row being in state ϕ; E is the sum of the vertex energies formed by the two states ϕ, ϕ' together with the horizontal arrows. From the definition of the partition function we have simply

$$Z(\beta) = \sum_{\phi_M} \cdots \sum_{\phi_1} T(\phi_1, \phi_M)\, T(\phi_M, \phi_{M-1}) \cdots T(\phi_2, \phi_1)$$
$$= \mathrm{Tr}[T^M] = \sum \lambda_j^M, \quad (2.1)$$

where λ_j are the eigenvalues of T. Since the elements of T are nonnegative, the Perron–Fröbenius theorem[1] guarantees that there is a positive maximum eigenvalue Λ which corresponds to an eigenvector having nonnegative components. We have simply

$$\lim_{M\to\infty} (1/M) \ln Z = \ln\Lambda. \quad (2.2)$$

We must thus formulate and solve the equation $T\Psi = \Lambda\Psi$.

It has been demonstrated[2] that horizontal periodicity and the ice rule are sufficient to ensure that $T(\phi,\phi') = 0$ unless ϕ and ϕ' have the same number n of down arrows, so that T decomposes into blocks of dimension $\binom{N}{n}, n = 0, 1, \ldots, N$. It is convenient to define an average polarization

$$y = 1 - 2n/N, \quad -1 \le y \le 1. \quad (2.3)$$

Since we need only solve the eigenvalue equation in each block separately, it is convenient to denote the corresponding eigenvector by $f(x_1, \ldots, x_n)$, where $1 \le x_1 \le x_2 \le \cdots \le x_n \le N$ denote the positions of the down arrows. We shall also denote the n-tuple simply by X. In a given matrix element, the first down arrow can occur in either the lower or the upper row, and so accordingly we can write

$$T = T_R + T_L, \quad (2.4)$$

where

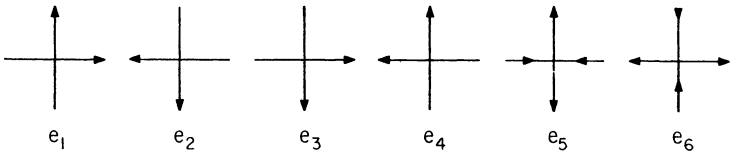

FIG. 1. The six allowed vertex configurations.

With M.L. Glasser and D.B. Abraham in J. Math. Phys. *13*, 887–900 (1972)

$$T_R(\mathbf{X},\mathbf{Y}) = \begin{cases} \neq 0, & \text{if} x_{i-1} \le y_i \le x_i, \quad i = 1,\dots,n, \\ 0, & \text{otherwise}, \end{cases}$$

$$T_L(\mathbf{X},\mathbf{Y}) = \begin{cases} \neq 0, & \text{if} x_i \le y_i \le x_{i+1}, \\ 0, & \text{otherwise}. \end{cases} \tag{2.5}$$

(The subscripts R, L refer to the direction of the horizontal arrows at the extremities.)

Because the zero of energy may be chosen freely and n-conservation implies that the number of type 5 vertices must be the same as the number of type 6 vertices on every row, there can be only four independent vertex energies. We take as these a linear combination of the vertex energies for the KDP[3] and F[4] models together with energies corresponding to the presence of direct (horizontal and vertical) fields:

$$\begin{aligned} e_1 &= \epsilon_2 - h - v, \quad e_2 = \epsilon_2 + h + v, \\ e_3 &= \epsilon_1 + \epsilon_2 - h + v, \\ e_4 &= \epsilon_1 + \epsilon_2 + h - v, \quad e_5 = e_6 = \epsilon_1. \end{aligned} \tag{2.6}$$

Now, because the configuration energies are linear in the vertex energies, for each element of the transfer matrix, we have $T = T^{\mathrm{KDP}} T^{\mathrm{F}} T^{H} T^{V}$.

For convenience we define the quantities

$$K_i = \beta\epsilon_i, \quad H = \beta h, \quad V = \beta v. \tag{2.7}$$

Then, by inspection, we find

$$\begin{aligned} T_R^V &= e^{NVy} = T_L^V, \\ T_R^H &= e^{NH} e^{2H\Sigma_1^n (y_i - x_i)} = e^{2NH} T_L^H(\mathbf{X},\mathbf{Y}). \end{aligned} \tag{2.8}$$

The transfer matrices for the F and KDP models are[3,4]

$$\begin{aligned} T_R^{\mathrm{F}}(\mathbf{X},\mathbf{Y}) &= T_L^{\mathrm{F}}(\mathbf{X},\mathbf{Y}) \\ &= \exp\left[-K_2\left(N - 2n + 2\sum_1^n \sum_1^n \delta(x_i - y_i)\right)\right] \\ T_R^{\mathrm{KDP}}(\mathbf{X},\mathbf{Y}) &= \exp K_1\left(-n + \sum_1^n (y_i - x_i) + 2\sum_1^{n-1} \delta(y_{i+1} - x_i)\right) \\ T_L^{\mathrm{KDP}}(\mathbf{X},\mathbf{Y}) &= \exp K_1\left(-N - n + \sum_1^n [y_i - x_i + 2\delta(y_i - x_i)]\right). \end{aligned} \tag{2.9}$$

We must now solve the eigenvalue equation

$$\Lambda f(\mathbf{X}) = \sum_R T_R(\mathbf{X},\mathbf{Y}) f(\mathbf{Y}) + \sum_L T_L(\mathbf{X},\mathbf{Y}) f(\mathbf{Y}), \tag{2.10}$$

where the sums denoted R and L are over all $1 \le y_1 \le \cdots \le y_n \le N$ consistent with the first or second condition in (2.5), respectively. The solution of (2.10) follows precisely the treatment of the ice model[2] to which we refer for details. We find that

$$\begin{aligned} \Lambda &= \Lambda_R + \Lambda_L, \\ \Lambda_R &= e^{N(Vy - K_2 + H)} \prod_{j=1}^n \frac{2\Delta - e^{K_1} - e^{ik_j + 2H}}{1 - \exp(ik_j - K_1 - 2H)}, \\ \Lambda_L &= e^{N(Vy - K_1 - K_2 - H)} \prod_{j=1}^n \frac{2\Delta - e^{-K_1} - e^{-ik_j - 2H}}{1 - \exp(-ik_j - K_1 - 2H)}, \end{aligned} \tag{2.11}$$

where

$$2\Delta = e^{K_1} + e^{-K_1} - e^{2K_2 - K_1}. \tag{2.12}$$

The numbers k_j are obtained by solving the n-equations

$$e^{ik_j N} = \prod_{\substack{i=1 \\ i \ne j}}^n B(k_j, k_i), \quad j = 1,\dots,n, \tag{2.13}$$

where

$$\begin{aligned} B(q,p)^{-1} &= B(p,q) = e^{-i\theta(p,q)} \\ &= \frac{1 + e^{4H + i(p+q)} - 2\Delta e^{2H + ip}}{1 + e^{4H + i(p+q)} - 2\Delta e^{2H + iq}}. \end{aligned} \tag{2.14}$$

When H is nonzero, the function θ is not real so that the numbers k_j are complex. What happens in this case has been explored briefly by Sutherland, Yang, and Yang,[5] but the details of their calculation are not available. In the remainder of this paper we shall assume that $H = 0$.

The important properties of the solution to (2.13), (2.14) which maximizes Λ for any n are:

(i) For $\Delta < 1$ the k_j are real.

(ii) For n even, if k_j is a root, then $-k_j$ is also a root.

(iii) It is assumed that for large even N the roots become densely distributed on some (finite or infinite) interval $(Q, -Q)$ with density $N\rho(k)dk$, where $\rho(k)$ is a smooth function.

(iv) For $\Delta = 1$, all the k_j vanish; i.e., $f(\mathbf{X}) = 1$.

Henceforth we shall adopt the notation

$$z(y) = \lim N^{-1} \ln[\max(\Lambda_R, \Lambda_L)] - Vy \tag{2.15}$$

so the free energy per vertex is given by

$$-\beta\mathfrak{F} = \max_y [z(y) + Vy]. \tag{2.16}$$

The discussions of the cases $\Delta \ge 1$ and $\Delta < 1$ are quite different, since in the former case the solution for $z(y)$ may be obtained by guile, avoiding the solution of (2.14). In general the k_j are complex but for $\Delta = 1$, from (iv) above, we have

$$z(y) = -K_2 + \max(0, -K_1) \tag{2.17}$$

independent of y. Now Eq. (2.17) implies: (i) $z(y)$ is convex and nonincreasing in K_1 and K_2, and thus is also convex and nonincreasing in the limit $N \to \infty$; (ii) by subtraction of ϵ_1 from the e_j, $z(y) \to z'(y) = z(y) + K_1$, where $z'(y)$ is convex in K_1 and K_2, nonincreasing in K_2 and nondecreasing in K_1. In the thermodynamic limit, the right-hand side of (2.17) is a lower bound on $z(y)$ for all Δ, because it can be achieved for $K_1 > 0$ by a single configuration which is a spiral band of type 1 vertices and a spiral band of type 2 vertices in the relative proportion $(1 + y) : (1 - y)$. These bands are separated by a ladder of alternating 5 and 6 vertices, but these make no contribution in the thermodynamic limit. The above argument is the same for $K_1 < 0$, with vertices 1 and 2 replaced by vertices 3 and 4. Using these results and the previous paragraph, we have the result:

Equation (2.17) is true for all y and all $\Delta \ge 1$.

It is clear that the system is completely frozen into homogeneous regions of vertex 1 and 4 when $\Delta \ge 1$,

the interfaces being composed of vertices 5 and 6. This complete ordering should be contrasted with the results for the Ising model.[6] Nagle[7] has given a rigorous proof of the freezing when $K_2 = 0$, using an argument due to Takahashi[8]; he also obtained a latent heat at $\Delta = 1$. The argument may be extended to cases with $K_2 \neq 0$, for which $\Delta = 1$ can be realized.

For $\Delta < 1$, (2.13) reduces, in the limit $N \to \infty$, to an integral equation for the density function $\rho(k)$, which we write in the form

$$1 = 2\pi\rho(p) - \int_{-Q}^{Q} \frac{\partial\theta(p,q)}{\partial p}\,\rho(q)dq, \tag{2.18}$$

where $Q(y)$ must be determined self-consistently by the condition

$$\tfrac{1}{2}(1-y) = \int_{-Q}^{Q} \rho(p)dp. \tag{2.19}$$

Once these equations have been solved for $\rho(p)$ and Q, the free energy may be determined. The calculation is simplified somewhat by noting that for $\Delta < 1$ either Λ_R or Λ_L vanishes in the thermodynamic limit, for

$$|1 - e^{ik+K_1}|^2 \left(\left| \frac{2\Delta - e^{K_1} - e^{ik}}{1 - \exp(ik + K_1)} \right|^2 - \left| e^{-K_1} \frac{2\Delta - e^{-K_1} - e^{ik}}{1 - \exp(-ik - K_1)} \right|^2 \right)$$

$$= 4(\cosh K_1 - 2\Delta + \cos k)\sinh K_1, \tag{2.20a}$$

whence it follows readily that

$$\begin{aligned} &|\Lambda_R| > |\Lambda_L| \quad \text{for } K_1 > 0, \\ &|\Lambda_R| < |\Lambda_L| \quad \text{for } K_1 < 0, \\ &|\Lambda_R| = |\Lambda_L| \quad \text{for } K_1 = 0. \end{aligned} \tag{2.20b}$$

Consequently, in the thermodynamic limit $z(y)$ is given by

$$z(y) = -K_2 + \max(0, -K_1) + \tfrac{1}{2}\int_{-Q}^{Q} \rho(q) \times \log\left(\frac{(2\Delta - \eta)^2 + 1 - (2\Delta - \eta)\cos q}{1 + \eta^2 - 2\eta\cos q} \right) dq, \tag{2.21}$$

where $\eta = e^{|K_1|}$. This is equivalent to the result obtained by Sutherland.[9]

Equation (2.18) occurs in the theory of the Heisenberg–Ising chain[10]; this is not surprising since T has been shown to commute with the Hamiltonian[11]

$$\mathcal{H}(\Delta) = -\sum_{j=1}^{n} (\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+ + \tfrac{1}{2}\Delta\sigma_j^z\sigma_{j+1}^z) \tag{2.22}$$

provided Δ is given, as before, by Eq. (2.12). It was first shown by Hulthén[12] and Walker[13] that there exist transformations which reduce the kernel of the integral equation (2.18) to difference form. This work was unified and completed by Yang and Yang,[10] whose notation we follow. The transformations $k \to \alpha(k)$ needed differ for the three regions $\Delta < -1$, $-1 < \Delta < 1$, and $\Delta \geq 1$.

For $|\Delta| < 1$ the wavenumbers k_j are restricted to lie in the interval $|k_j| < (\pi - \mu)$, where

$$\cos\mu = -\Delta, \quad 0 < \mu < \pi. \tag{2.23}$$

The transformation which reduces the equation to difference type is

$$e^{ik} = (e^{i\mu} - e^{\alpha})/(e^{\alpha}e^{i\mu} - 1). \tag{2.24}$$

Even under this transformation we still have two coupled complicated integral equations to solve. In the case $y = 0$, which is applicable in the absence of a vertical external field, the quantity Q becomes infinite and the equation can be solved by Fourier analysis. Therefore, from now on we shall restrict ourselves to the cases $H = 0$, $V = 0$, where the free energy is given by $z(0)$. The important features of the behaviour in a vertical field can be determined by the means used for the F and KDP models. For $y = 0$ the density is

$$\rho(k)\,(dk/d\alpha) = (\tfrac{1}{4}\mu)\,\operatorname{sech}(\pi\alpha/2\mu), \quad |\Delta| < 1. \tag{2.25}$$

For $\Delta < -1$ the appropriate transformation is

$$e^{ik} = (e^{\lambda} - e^{-i\alpha})/(e^{\lambda - i\alpha} - 1), \tag{2.26}$$

where

$$\cosh\lambda = -\Delta, \quad 0 < \lambda < \infty. \tag{2.27}$$

In the case $y = 0$ we have $|\alpha| < \pi$ and the equation can be solved by Fourier series, leading to

$$\rho(k)\frac{dk}{d\alpha} = \frac{\pi}{4\lambda}\sum_{-\infty}^{\infty} \operatorname{sech}\left(\frac{\pi(\alpha + 2\pi n)}{2\lambda}\right). \tag{2.28}$$

In this case the density is closely related to the Jacobian elliptic function[14] cn, and, as we shall point out again later, there seems to be an ill-defined but pervasive connection between the ferroelectric problems and the theory of elliptic functions which may well have been finally established by Baxter.[15]

The free energy is given by (2.16), where $z(y)$ is given by (2.22) for $\Delta < 1$. Yang and Yang[10] have proven that, for $1 \geq y > 0$, $\rho(q)$ considered as a function of Δ and y is real analytic in Δ and y, which gives the following result:

> $z(y)$ is real analytic in the temperature and in y provided
>
> $0 < y \leq 1$ and $\Delta < 1$.

The case $y = 0$, which is pertinent if $V = 0$, is exceptional in this respect. For $\Delta < 1$ the kernel of the integral is not analytic in Δ at $\Delta = -1$. In the remainder of this paper we shall discuss this case. Our first conclusion is that singular behavior is only to be expected at $\Delta = \pm 1$. It is important, therefore, to decide what values of Δ can be realized on the real positive temperature axis for a given assignment of vertex energies. This is summarized in the following easily proven theorem:

Theorem: If the temperature T is real and positive, then $\eta \geq 1$ and:

(1) For no values of ϵ_1 and ϵ_2 can both $\Delta = +1$ and $\Delta = -1$ be realized as T is varied,

(2) If $\epsilon_2 > \max(0, \epsilon_1)$, then $-\infty < \Delta < \tfrac{1}{2}$ for real T, whereas if $\epsilon_2 < \max(0, \epsilon_1)$, $\tfrac{1}{2} < \Delta < \infty$. If $\epsilon_2 =$

$\max(0, \epsilon_1)$, then $0 \le \Delta < \frac{1}{2}$; there is no singular behavior in this case.

3. PROPERTIES OF THE FREE ENERGY

Since both $\rho(k)$ and the argument of the logarithm in Eq. (2.21) are analytic with respect to Δ and η in the regions $|\Delta| < 1$ and $\Delta < -1$, critical behavior in the free energy can be expected only for $\Delta = \pm 1$. From an examination of the $\Delta = \pm 1$ contours in the (K_1, K_2) plane shown in Fig. 2, we can divide the plane into two broad regions, which we label I and II. Region I, in which, as will be seen, the model is antiferroelectric in character, contains the F model, and region II, in which the model is ferroelectric, we have the KDP model, both of which have been studied in detail by Lieb.[3,4] In Addition, there are two singular cases: the IKDP model discussed by Glasser[16] and the IF model, which we shall consider below. In addition to these models, which correspond to rays in the $K_1 - K_2$ plane, there are the ice model ($K_1 = K_2 = 0$) and a limiting case studied by Wu,[17] where $\Delta = 0$, which we shall not consider further.

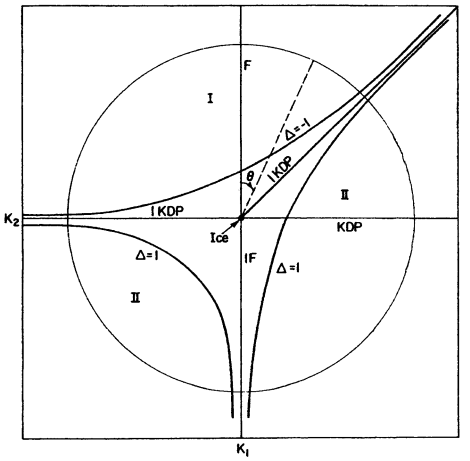

FIG. 2. Classification of models in the scaled (ϵ_1, ϵ_2) plane $(K_i = \beta\epsilon_i)$. I and II are the regions $\pi/2 > \theta > -\pi/4$ and $-3\pi/2 < \theta < -\pi/4$, respectively.

The behavior of Δ as a function of inverse temperature is shown in Fig. 3 (for the IF model Δ attains 1 at $\beta = \infty$). We define a transition temperature T_0 by the condition $\Delta = \pm 1$; the behavior of T_0 as a function of the angle θ shown in Fig. 2 is given schematically in Fig. 4.

It is convenient to introduce the parameters

$$e^{i\varphi_0} = (1 + \eta e^{i\mu})/(e^{i\mu} + \eta), \qquad 0 \le \varphi_0 \le \mu, \ |\Delta| < 1, \tag{3.1}$$

$$e^{\theta_0} = (1 + \eta e^{\lambda})/(e^{\lambda} + \eta), \qquad 0 \le \theta_0 \le \lambda, \ \Delta < -1. \tag{3.2}$$

Then in the "high temperature" regime the free energy of our model may be expressed, by inserting (2.25) into (2.21), as

$$\mathfrak{F} = \epsilon_2 + \max(0, \epsilon_1) - \tfrac{1}{4} kT \int_{-\infty}^{\infty} \frac{d\alpha}{\cosh \pi\alpha} \times \ln\left(\frac{\cosh(2\mu\alpha) - \cos(2\mu - \varphi_0)}{\cosh(2\mu\alpha) - \cos\varphi_0}\right), \qquad T > T_0, \tag{3.3}$$

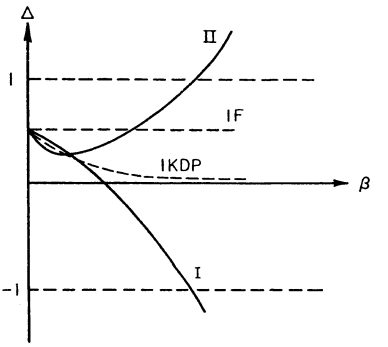

FIG. 3. Behavior of the parameter Δ as a function of inverse temperature for the models of Fig. 2.

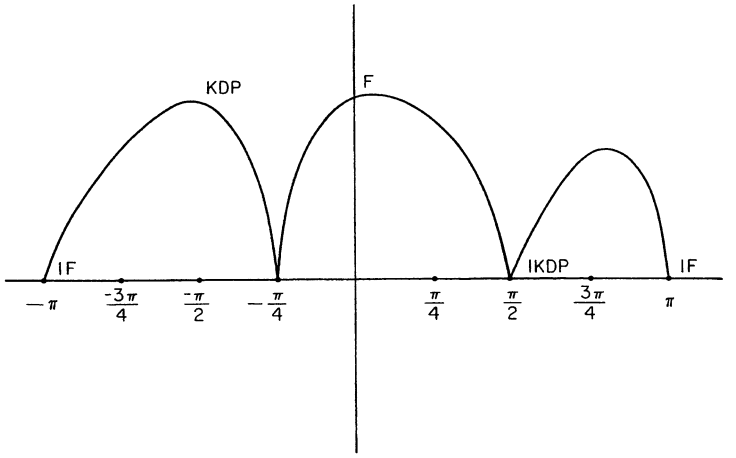

FIG. 4. Behavior of the transition temperature as a function of the angle θ of Fig. 2.

which is applicable to both regions I and II, which we discuss separately.

For region II we have that $\Delta = 1$ corresponds to $\mu = \pi$. At $\mu = \pi$ the argument of the logarithm in (3.3) becomes unity, so that the integral vanishes and the high temperature free energy joins continuously to the "low temperature" value given by (2.17). Therefore, we evidently have a first-order phase transition to a ferroelectrically ordered low-temperature phase. Since $\mathfrak{F}$ depends analytically on η about η_0, any singular behavior must be due to the dependence of the high temperature free energy on μ, since

$$\frac{d\mu}{d\Delta} = \csc\mu, \tag{3.4}$$

which is infinite at $\mu = \pi$. Indeed, a simple calculation gives

$$\mathfrak{F} = \frac{(\pi-\mu)^2}{4(\eta-1)} + \frac{(\pi-\mu)^3}{3(\eta-1)\pi} + O[(\pi-\mu)^4], \qquad T > T_0. \tag{3.5}$$

The singular part of the specific heat at vanishing vertical polarization is

$$C_0 \cong \frac{k}{4(\eta-1)\pi}\left(\frac{2\epsilon_1 \sinh K_1 - (2K_2 - K_1)e^{(2K_2-K_1)}}{kT_c}\right)^{3/2} \times\left(\frac{T}{T_c}-1\right)^{-1/2}. \tag{3.6}$$

The first-order phase transition in this case is unusual in that the low and high temperature-free energy functions cross where the latter has a vertical tangent as a function of temperature. For the special case of the KDP model, (3.6) reduces to give the behavior obtained previously.[3] This case will be treated in more detail in Sec. 4. This concludes the study of the free energy in the ferroelectric region II.

In the case of the IF model, for which $\eta = 1$, $e^{2K_2} < 1$, which represents a singular case in region II, we have $T_0 = 0$ and find for the expansion of the free energy about $\mu = \pi$

$$\mathfrak{F} \cong -\tfrac{1}{2}\, kT(\pi-\mu)[1 + \tfrac{1}{2}(\pi-\mu) + \cdots]. \tag{3.7}$$

From this we find for the internal energy

$$U \cong \tfrac{1}{2}\,|\epsilon_2|\, e^{2K_2}(\csc\mu)[1 + (\pi-\mu) + \cdots]. \tag{3.8}$$

Since, in this case

$$e^{2K_2} = 1 - \Delta, \tag{3.9}$$

we have

$$U \cong \tfrac{1}{2}\,|\epsilon_2|(\pi-\mu) + O[(\pi-\mu)^2], \tag{3.10}$$

and

$$C_0 \cong 2^{-1/2}|\epsilon_2|^2/(kT)^2. \tag{3.11}$$

In this case the evident vanishing of the latent heat means that there is a second-order phase transition at $T = 0$.

In region I, which includes the antiferroelectric F model, (3.3) again describes the high-temperature region $T > T_0$, but $T = T_0$ now corresponds to $\mu = 0$. This gives rise to an interesting phenomenon. Consider the function $H(\mu)$ defined by the integral

$$H(\mu) = \int_{-\infty}^{\infty} d\alpha\, \mathrm{sech}(\pi\alpha) f(\alpha, \mu). \tag{3.12}$$

The singularities of the integrand are simple poles due to $\mathrm{sech}(\pi\alpha)$ evenly spaced along the imaginary axis in the α plane together with the singularities of $f(\alpha, \mu)$ for positive real μ, which we represent as the blobs in Fig. 5. The location of these singularities depends on μ. (We assume f is real analytic, and so by the Schwartz reflection principle the singularity set of f is invariant under complex conjugation.) Let us now suppose that the singularities of f are rational in μ. As we allow μ to circle the origin in the μ plane, the blobs, which may also change shape, will circle the origin in the α plane. To avoid integrating through a singularity, we must deform the contour of integration more and more, until it gets pushed up against the imaginary axis. If the singularity set of f is

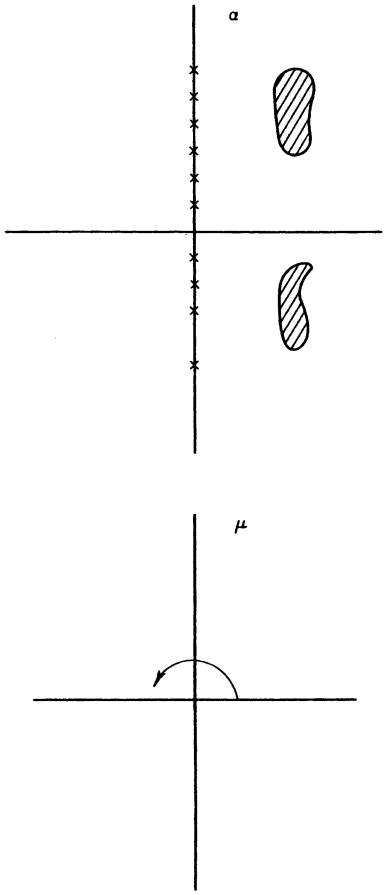

FIG. 5. Singularity structure for the hypothetical function $f(\alpha, \mu)$.

With M.L. Glasser and D.B. Abraham in J. Math. Phys. *13*, 887–900 (1972)

wider than the spacing of the poles along the imaginary axis, the contour will certainly become pinched, thereby forcing us to integrate through a singularity and causing there to be a singularity in $H(\mu)$ in the μ plane. In the case of the integral in (3.3) for small positive μ, the singularities of the logarithm form several lines of branch points. As we circle the origin in the μ plane these lines move in a complicated way determined in part by the dependence of φ_0 on μ. By the implicit function theorem, however, this dependence can be shown to be analytic in a neighborhood of $\mu = 0$, where $\varphi_0 = 0$. Thus for small μ we can ignore the presence of φ_0. Therefore, these lines of singularities simply rotate synchronously with μ, and, when μ approaches any small negative rational multiple of π, a pinch will occur. This shows that, at least in a small neighborhood of $\mu = 0$, the negative real axis forms a natural boundary (line segment having a dense set of singularities) with end point at $\mu = 0$. Since for larger μ the dependence of φ_0 on μ becomes more complex, it may happen that the natural boundary may disappear or take on some complicated form away from the origin in the μ plane. In Appendix A, however, we show that this does not happen and that the entire negative real axis is a natural boundary for the high temperature-free energy in region I. It may also happen, of course, that the function f in the integrand of $H(\mu)$ has zeros which coincide with the poles of $\operatorname{sech}(\pi\alpha)$ in which case the contour will not be pinched. In Appendix B we show that this actually happens in the case of the KDP and IKDP models, but for no others.

We may formally expand (3.3) in even powers of μ, where we take into account the fact that φ_0 is odd and analytic in μ; it is shown in Appendix D that the coefficients are all finite. However, as we have just demonstrated, $\mu = 0$ is a nonisolated singularity so that this series must have vanishing radius of convergence. We next note that Δ is analytic with respect to T about $T = T_0$, and, as can be proven from the implicit function theorem, $\mu^2 = [\arccos(-\Delta)]^2$ is an analytic function of Δ about $\Delta = -1$. { This surprising fact also follows from the identity $\arccos z = [2(1-z^2)^{1/2}/(1+z)]\,{}_2F_1[\frac{1}{2}, 1; \frac{3}{2}; (z-1)/(z+1)]$.} The free energy in region I is therefore infinitely differentiable, but nonanalytic as $T \to T_0^-$.

To characterize the thermodynamic behavior of the system completely, we must examine the behavior of the free energy as $T \to T_0^-$. From (2.28) and (2.21) we have in the low temperature region, where $\Delta < -1$

$$\mathfrak{F} = \epsilon_2 + \max(0, \epsilon_1) - \tfrac{1}{2} kT(\lambda - \theta_0) - kT \sum_{n=1}^{\infty} \frac{e^{-\lambda n} \sinh n(\lambda - \theta_0)}{n \cosh n\lambda}. \quad (3.13)$$

We note that this expression is nonsingular below $T_0(\lambda = 0)$ down to $T = 0(\lambda = \infty)$. Next we see that (3.8) and (3.3) agree at $T = T_0$ (where $\lambda = \theta_0 = 0$, $\mu = \varphi_0 = 0$). Finally, as is shown in Appendix A, (3.8) is the analytic continuation of (3.3) onto the imaginary μ axis. The entire free energy is thus described in terms of a single function, infinitely differentiable, but nonanalytic at $T = T_0$ and nonsingular at every other real temperature. We therefore conclude that in region I the system undergoes an infinite order phase transition. Since at low temperatures vertices 5 and 6, of which there must be an equal number, are favored, this transition is to an antiferroelectrically ordered state and occurs without any thermodynamic anomalies. To remove any doubt on these matters, we present in Appendix A a detailed calculation of the smooth matching of the high and low temperature-free energies at T_0.

We come finally to the IKDP model which separates region I from region II. In this case we have either $K_1 = K, K_2 = 0$ or $K_1 = K_2 = K \geq 0$ and $0 \leq \Delta \leq \frac{1}{2}$, which corresponds to $\frac{1}{2}\pi < \mu \leq 2\pi/3$, and $\varphi_0 = 2\pi - 3\mu$. Thus the system is essentially always in the "high temperature" region and the free energy is

$$\mathfrak{F} = \epsilon - \tfrac{1}{4} kT \int_{-\infty}^{\infty} d\alpha \operatorname{sech}(\pi\alpha) \ln\left(\frac{\cosh(2\mu\alpha) - \cos(5\mu)}{\cosh(2\mu\alpha) - \cos(3\mu)}\right) \quad (3.14)$$

As shown in Appendix B, the integral in this case can be evaluated in terms of elementary functions and we have

$$\mathfrak{F} = 2\max(0, \epsilon) + kT \ln[(\pi/2\mu) \sin\mu \tan(\pi^2/2\mu)]. \quad (3.15)$$

It will be seen below that (3.15) is the analytic continuation in ϵ of the free energy for KDP. These two models merge continuously at $T = \infty$. It is seen that (3.15) has no singularity for any real T. Because of the behavior of the $\Delta = \pm 1$ contours in Fig. 2, however, we define T_0 to be zero in this case.

This concludes our discussion of the thermodynamic properties of the general model in the absence of external fields, except to point out that as $T \to \infty$ in any special case we obtain the ice model for which

$$z(0) = \tfrac{3}{2} \ln 3. \quad (3.16)$$

4. DETAILED ANALYTIC STRUCTURES FOR THE KDP AND F MODELS

The analytic properties of the Onsager solution for the free energy of the two dimensional Ising model have been studied in detail by Majumdar.[18] For comparison with the results for the ferroelectric models we have extended his results to obtain the behavior of the free energy in the complex temperature plane. This is shown in Fig. 6. The characteristic structure of this and succeeding diagrams arises in the following way. The partition function or free energy is most conveniently expressed in terms of an activity of the form $z = \exp(\beta J)$ and in the complex z plane will have a relatively simple analytic structure. When the logarithm is taken to get the analytic structure in the β plane, each singularity z_0 in the z plane becomes a sequence of singularities $\beta_0 + 2k\pi i$, $k = 0, \pm 1, \cdots$, which lie along a line parallel to the imaginary β axis. Finally, in taking the reciprocal to obtain the behavior in the temperature plane, lines which extend to infinity go into circles passing through $T = 0$, and the analytic structure consequently has a circular geometry. We note in Fig. 6 in the complex temperature Riemann structure for the Ising model a branch cut begins at $T = T_0$ and extends down to $T = 0$. As Majumdar showed this is due to the fact that the analytic continuation of the free energy from the high- to the low-temperature region does not remain real valued, but one must average the results taken above and below the branch cut in order to ob-

tain the physical result. This is similar to the situation for the F-like models in region I and is due to the fact that the free energy for real temperature depends on $|T - T_0|$, which is not an analytic relationship.

KDP Model

The free energy for the KDP model is given (up to an additive constant) by Eq. (B. 12). If we let $z = \mu/\pi$, we have $\Delta = -\cos\pi z$ and $\Delta = \frac{1}{2}e^{\beta\epsilon}$. Note that, for $T = \infty$, $z = \frac{2}{3}$ and (B. 12) gives $\frac{3}{2}\ln(\frac{4}{3})$, which is the residual entropy of square ice.[2]

The analytic structure below T_0 is trivial, and so we consider only the Riemann structure of the high-temperature free energy. The singularities of $\mathfrak{F}$ in

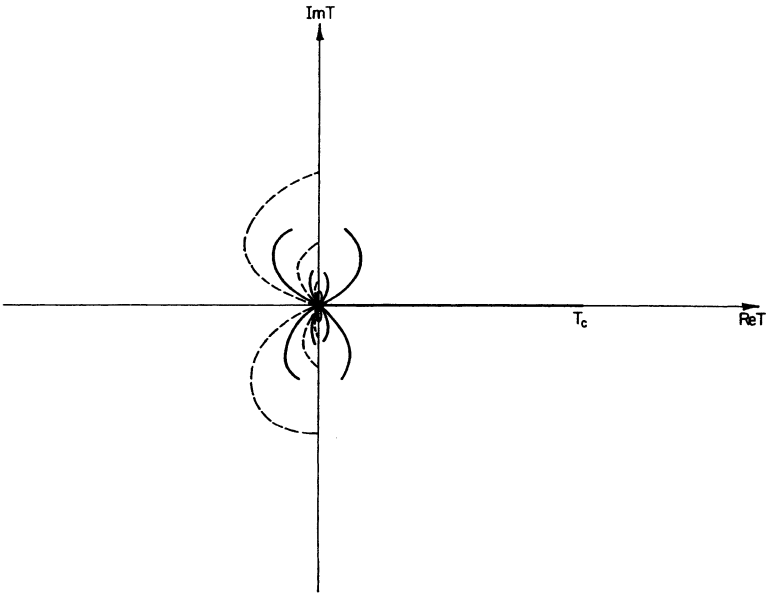

FIG. 6. Riemann structure for the two-dimensional Ising model in the complex temperature plane. The lines denote logarithmic branch cuts.

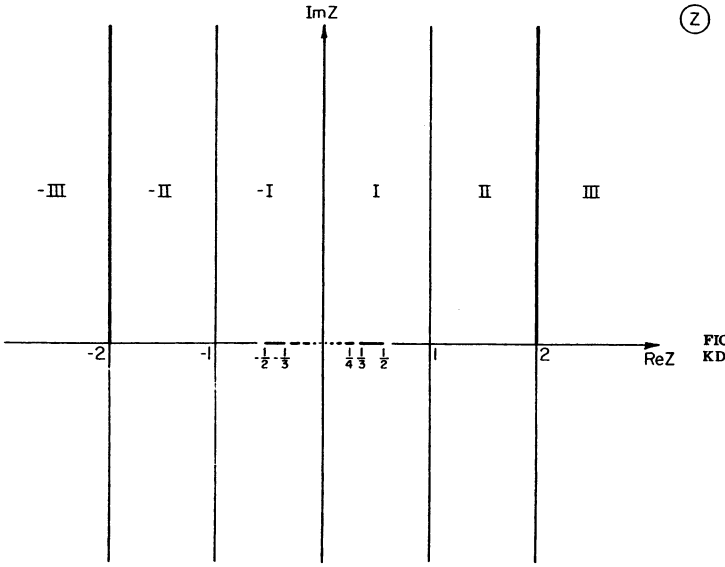

FIG. 7. Riemann structure for the KDP model in the complex z-plane.

the z plane are logarithmic branch points at $z = 1/n$, $n, n = \pm 2, \pm 3, \cdots$, and we have branch cuts $\pm(1/2|n|, 1/2(|n| + 1|))$ and cuts starting at $z = n$ which we take parallel to the imaginary z axis as shown in Fig. 7. $z = 0$ is an accumulation point of branch points and is an essential singularity. Next we note that each strip of unit width as indicated in the z plane maps onto an entire Riemann sheet in the Δ plane. We label the corresponding sheets Δ_N, $N = \pm \mathrm{I}, \pm \mathrm{II}, \cdots$. These sheets are connected along branch lines $(\pm 1, \pm \infty)$ as shown schematically in Fig. 8. The line $z = n$ corresponds to the two edges of the positive (negative) cut if n is odd (even). The small branch cuts on strips $\pm$ I of the z plane map into similar cuts $(-\cos(\pi/2|n|), -\cos[\pi/(2|n| + 1)])$ which occurs on Δ_I and Δ_{-I} only. The remaining Δ-structure is free of additional singularities. A small circle centered at $z = n\pi$ maps into a small circle about $\Delta = \pm 1$, and tracing the circle once in the positive sense in the z plane is equivalent to circling $\Delta = \pm 1$ twice in the positive sense.

The sheets $\Delta_{\pm 1}$ are each connected (along the small branch cuts) to a countable number of additional Δ planes which we denote $\Delta_{\pm \mathrm{I}}^{(n)}$. On these planes the values of $\mathfrak{F}$ differ by $n\pi i$ from its values on $\Delta_{\pm \mathrm{I}} \equiv \Delta_{\pm \mathrm{I}}^{(0)}$. On $\Delta_{\mathrm{I}}^{(0)}$, by circling $\Delta = 1$ clockwise, we go to $\Delta_{\mathrm{II}} \equiv \Delta_{\mathrm{II}}^{(0)}$ and again circling $\Delta = 1$ return us to $\Delta_{\mathrm{I}}^{(0)}$. The same thing happens for $\Delta = -1$. However, if on Δ_{II} we go to -1 and circle this point we do not return to Δ_{I}, but spiral onto another countable set of Riemann sheets $\Delta_{\mathrm{II}}^{(n)}$ on which the values of $\mathfrak{F}$ differ from those on $\Delta_{\mathrm{II}}^{(0)}$ by $n\pi i$. This same situation occurs for all the remaining sheets $\Delta_N \equiv \Delta_N^{(0)}$. Thus, we have a doubly countable infinite collection of Riemann sheets $\Delta_N^{(n)}$, $N = \pm \mathrm{I}, \pm \mathrm{II}, \cdots$, $n = 0, \pm 1, \pm 2, \cdots$. For $N = \pm \mathrm{I}$, the $\Delta_N^{(n)}$ are joined along the small branch cuts, and for $N \neq \pm \mathrm{I}$ they are joined along the long branch cuts.

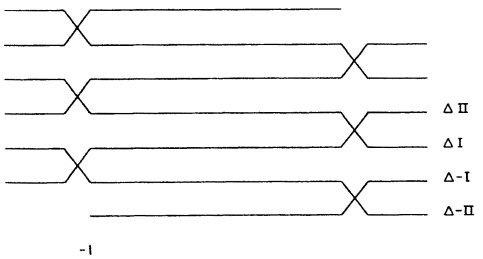

FIG. 8. Connectivity of the Δ sheets in the Riemann structures for the ice models.

Next we consider the Riemann structure for $\mathfrak{F}$ as a function of β. As indicated above, the analytic structure in the β-plane is periodic with period $2\pi i/\epsilon$, so we need only look at the principal strip $0 \leq \mathrm{Im}\beta < 2\pi/\epsilon$. Each Riemann sheet $\Delta_N^{(n)}$ corresponds to a Riemann sheet $\beta_N^{(n)}$. Of these, $\beta_{\mathrm{I}}^{(0)}$ and $\beta_{\mathrm{I}}^{(0)}$ are typical and are shown in Fig. 9. $\beta_{\mathrm{I}}^{(0)}$ is shown and $B_{\mathrm{II}}^{(0)}$ differs only in the absence of the cuts labeled (3) and (4). The connectivity as regards the various sheets exactly mirrors that for the $\Delta_N^{(n)}$ except going from $\Delta = 1$ to $\Delta = -1$ means leaving $\beta = \ln(2/\epsilon)$ along the negative real axis and returning to $\ln(2/\epsilon) + \pi i/\epsilon$ parallel to the positive real axis. Finally, the behavior in the complex T plane is shown in Fig. 10.

F Model

For clarity we repeat here for the F model the general considerations applied to region I.

The solution for the free energy of the F model can be written (for $T > T_c$)

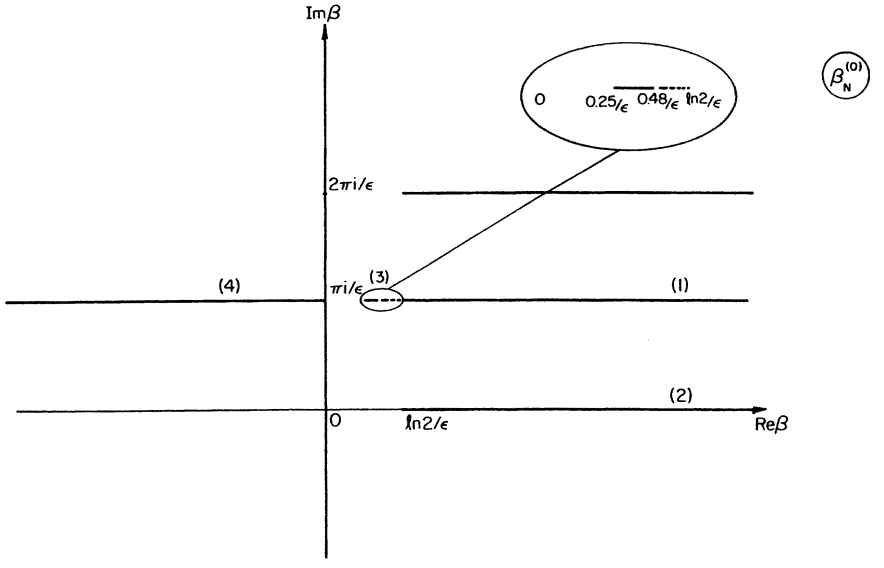

FIG. 9. Riemann structure for the KDP model in the complex β plane.

$$\Phi \equiv -\frac{F}{kT} = -\beta\epsilon + \frac{1}{8\mu}\int_{-\infty}^{\infty} dx\ \operatorname{sech}\left(\frac{\pi x}{2\mu}\right) \times \ln\left(\frac{\cosh x - \cos 2\mu}{\cosh x - 1}\right),$$

$$\Delta = -\cos\mu = 1 - \tfrac{1}{2}e^{2\beta\epsilon}. \qquad (4.1)$$

Following the procedure in Ref. 16, Eq. (12), we find

$$I = \int_0^{\infty} dx\ \operatorname{sech}\left(\frac{\pi x}{2\mu}\right) \ln\left(\frac{\cosh x - \cos 2\mu}{\cosh x - 1}\right) = 2\mu \int_0^{\infty} \frac{dx}{x}\ \operatorname{sech}\mu x[\coth\pi x(1 - \cosh xy) + \sinh xy], \qquad (4.2)$$

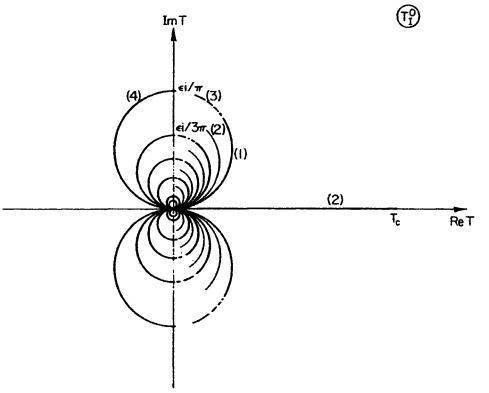

FIG. 10. Riemann structure for the KDP model in the complex temperature plane.

where $y = 2(\mu - n\pi)$ and $n\pi \le \mathrm{Re}\mu < (n+1)\pi$. Equation (4.2) can be rewritten

$$I = 4\mu \int_0^{\infty} \frac{dx}{x}\ \frac{\sinh(\mu - n\pi)x}{\cosh\mu x}\ \frac{\sinh[(n+1)\pi - \mu]x}{\sinh\pi x}, \qquad n\pi \le \mathrm{Re}\mu < (n+1)\pi, \qquad (4.3)$$

or

$$I = \begin{cases} 4\mu \int_0^{\infty} \frac{dx}{x}\ \tanh\mu x\ \frac{\sinh(\pi - \mu)x}{\sinh\pi x}, & 0 \le \mathrm{Re}\mu < \pi, \qquad (4.4a) \\ 4\mu \int_0^{\infty} \frac{dx}{x}\left(\frac{\tanh\mu x}{\tanh\pi x} - 1\right) \sinh[(2\pi - \mu)x], & \pi \le \mathrm{Re}\mu < 2\pi. \qquad (4.4b) \end{cases}$$

The first integral in (4.4) converges for all μ in the strip $0 \le \mathrm{Re}\mu < \pi$ and, therefore, defines an analytic function $\Phi_1(\mu)$. The singularities of the integrand are poles at the points $x_0(k) = ik$, $x_1(k) = (2k+1)\pi i/2\mu$, $k = 0, \pm 1, \pm 2, \cdots$ (excluding $x = 0$). The corresponding residues are

$$x_0(k) : \frac{1}{k\pi i}\ \frac{\sin^2 k\mu}{\cos k\mu},$$

$$x_1(k) : \frac{2(-1)^{k+1}}{\pi i(2k+1)} \cot\left((2k+1)\frac{\pi^2}{2\mu}\right). \qquad (4.5)$$

As μ moves counterclockwise along a semicircle from the right half-plane to $-\mu$ in the left half-plane, the pair of poles $x_1(k) = -x_1[-(k+1)]$ also exchange positions along semicircular paths. In doing this, the poles $x_1(k)$ break through the positive real axis (in the x plane), which we can deform into the positive real axis together with small counterclockwise circles

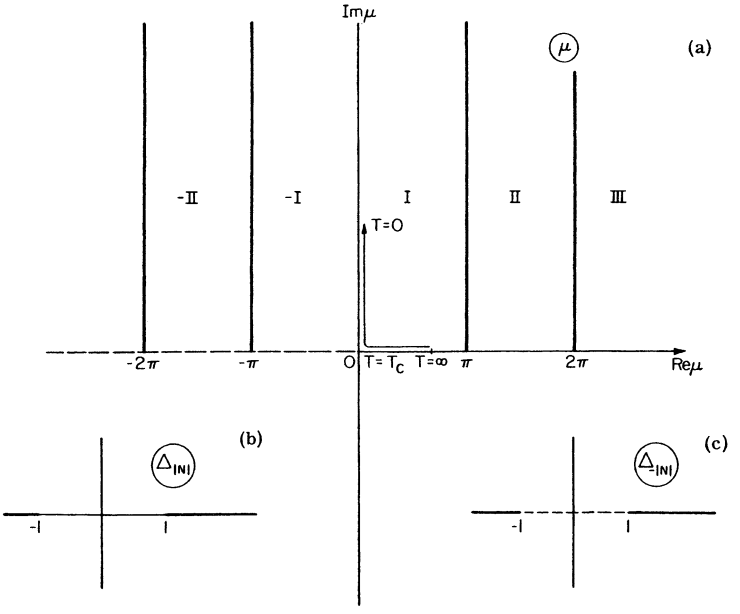

FIG. 11. Riemann Structure for the F model in the complex μ plane.

about the point $x_1(k)$. By noting that the pole structure remains completely unchanged, we have

$$\Phi_1(-\mu) = \Phi_1(\mu) + 2\pi i \sum \text{Residue at } \frac{k\pi i}{2\mu}$$
$$= \Phi_1(\mu) + 4 \sum_{k=1,\text{odd}}^{\infty} \frac{(-1)^{(k+1)/2}}{k} \cot\left(\frac{k\pi^2}{2\mu}\right)$$
$$= \Phi_1(\mu) + 4\Phi_2(\mu). \qquad (4.6)$$

It is interesting to note that the series in (4.6) is closely related to the elliptic function[14] dn. Thus, we can continue $\Phi_1(\mu)$ from the strip $0 \le \mathrm{Re}\mu < \pi$ to the strip $-\pi < \mathrm{Re}\mu \le 0$. Next we note that $\Phi_2(\mu)$ is a uniformly convergent series everywhere off the real μ axis. However, for μ real $\Phi_2(\mu)$ has a pole at every rational multiple of π, $m\pi/n$, where n is odd. These points are dense on the real line so that any expansion of $\Phi_2(\mu)$ in a power series about any real point will have zero radius of convergence, i.e., $\Phi_2(\mu)$ has a natural boundary along the real axis.

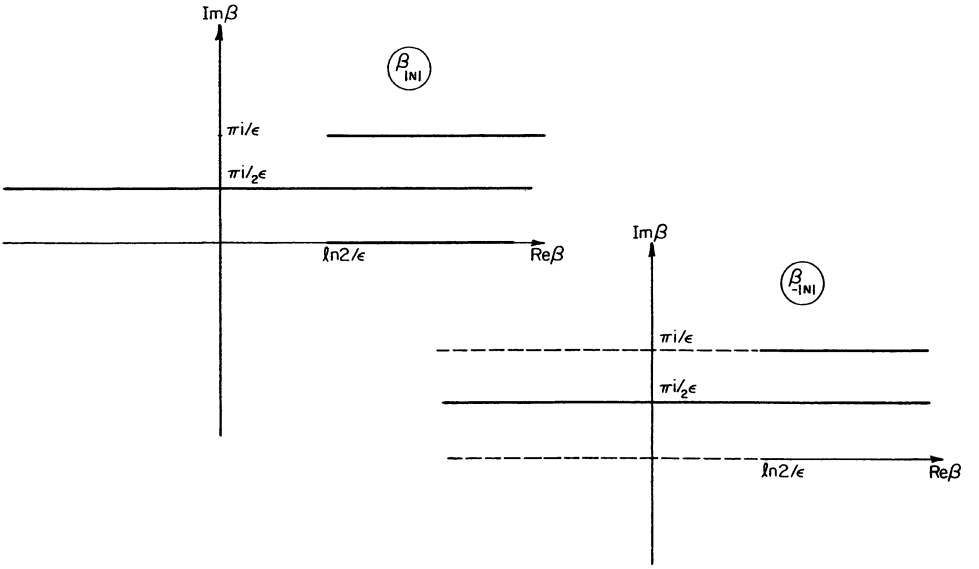

FIG. 12. Riemann Structure for the F model in the complex β-plane.

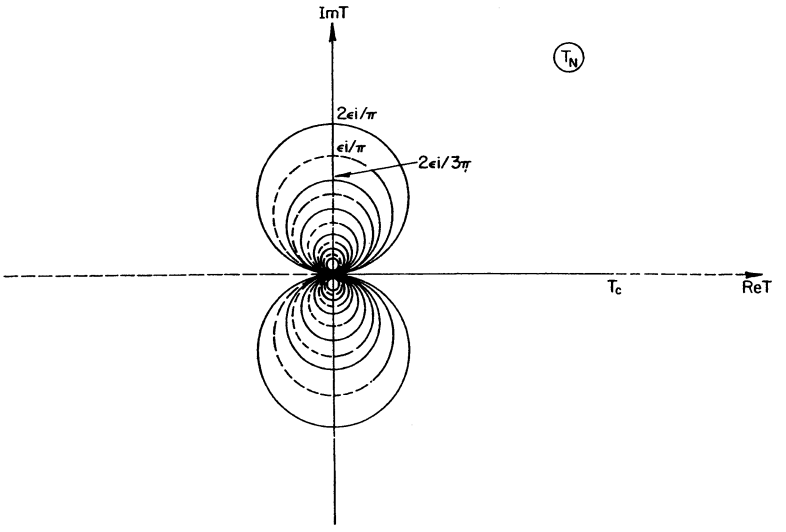

FIG. 13. Riemann structure for the F model in the complex temperature plane.

Since the same argument applied to each of the representations (4.3) leads to the same conclusion, we see that $\Phi(\mu)$ is analytic everywhere in the μ plane except for a natural boundary along the negative μ axis as shown in Fig. 11(a). Again, since $\Delta = -\cos\mu$, each strip of the μ plane of width π parallel to the imaginary axis maps into an entire Reimann sheet of the Δ-Riemann structure. These are connected as indicated in Fig. 8. Each Riemann sheet Δ_N has branch cuts $(-1, -\infty)$, $(1, \infty)$. Thus, if one begins at $\Delta_I = 0$ and circles $\Delta_I = 1$, one goes onto Δ_{II}. By circling $\Delta = 1$ again, one returns to Δ_I or by then circling $\Delta_{II} = -1$ goes to Δ_{III}, etc. Other than these branch cuts, the sheets Δ_N, $N = I, II, \cdots$, are free of singularities. However, if we begin at Δ_I (physical sheet above T_c) and circle -1, we go to Δ_{-I}. Δ_{-I} has a natural boundary along the interval $[-1, 1]$, which cannot be crossed. By circling the entire interval, we go to Δ_{-II}, Δ_{-III}, etc., all of which have the same structure as Δ_{-I}. These two types of Riemann sheets are shown in Fig. 11(b), (c). Once again, the β-Riemann surface has the same singularity structure as the Δ-surface except that the behavior in the fundamental strip is repeated periodically throughout each sheet. The cuts $(\pm 1, \pm\infty)$ become $(-\infty + \pi i/2\epsilon, \infty + \pi i/2\epsilon)$ and $\ln(2/\epsilon) < \beta < \infty$. The natural boundary $(-1, 1)$ maps into $(-\infty, \ln(\epsilon/2))$. The resulting structures are shown in Fig. 12. Finally, the Riemann structure in the temperature plane is shown in Fig. 13.

Finally, we must consider the low temperature-free energy for the F model. In the original work[4] this was described by a different analytic expression than (4.1). However, for $T < T_c$, we have $\Delta < -1$, and μ becomes pure imaginary, $\mu = i\lambda$. Now if in (4.4) we set $\mu = i\lambda + \epsilon$ and take the limit as $\epsilon \to 0$, we find

$$\Phi = -\beta\epsilon + \tfrac{1}{2}\,\mathrm{Im}\int_{-\infty}^{\infty}\frac{dx}{x}\,\coth\pi x\,\tan\lambda x\,e^{i\lambda x}, \qquad (4.7)$$

where the slash on the integral sign denotes that we take the Cauchy principal part in integrating past the singularities of the integrand. By closing the contour of integration in the upper half-plane, we obtain, by summing the residues at the singularities of $\coth\pi x$, ni, being careful to include only half the residue of the singularity at $x = 0$,

$$\mathrm{Re}\Phi = -\beta\epsilon + \tfrac{1}{2}\lambda + \sum_{n=1}^{\infty}\frac{1}{n}\,\tanh n\lambda\,e^{-n\lambda} \qquad (4.8)$$

which is precisely the old expression. Therefore, the imaginary axis in the μ plane describes the low temperature behavior as indicated in Fig. 11(a). Once again the series in (4.8) is related to an elliptic function.[14]

ACKNOWLEDGMENT

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APPENDIX A

The function $\Phi(\mu)$ is defined by

$$\Phi(\mu) = \frac{1}{4}\int_{-\infty}^{\infty}\frac{dx}{\cosh(\pi x)}\,\log\left(\frac{\cosh(2\mu x) - \cos(2\mu - \phi_0)}{\cosh(2\mu x) - \cos\phi_0}\right), \qquad (A1)$$

where $\phi_0(\mu)$ is defined by

$$e^{i\phi_0(\mu)} = (1 + \eta e^{i\mu})/(\eta + e^{i\mu}) \qquad (A2)$$

as a function of the complex variable μ which we write as

$$\mu = \mu_1 + i\mu_2. \qquad (A3)$$

In the range $-1 < \Delta < 1$, which corresponds to $0 < \mu_1 < \pi$, Eq. (2.21) gives

$$z(0) = -K_2 + \max(0, -K_1) + \Phi(\mu). \qquad (A4)$$

Clearly there is a *single independent* variable in the physical problem; obvious choices for this are μ or T. Thus η depends on T, or indirectly on μ. Several remarks are relevant in this connection.

(1) For the F and IF cases, the problem is much more simple since $\eta = 1$ for all T; thus $\phi_0(\mu) \equiv 0$. Theorem 1 below discusses the analytic properties in the μ plane for this case.

(2) For the KDP and IKDP cases, the function $\Phi(\mu)$ can be evaluated in terms of elementary functions.[16]

(3) The physical properties of the model are evidently all obtained by considering a small neighborhood of the real positive temperature axis.

Theorem 1: Consider the case $\phi_0 \equiv 0$:

(1) $\Phi(\mu)$ can be analytically continued to the entire μ plane except the line $\mu_2 = 0, \mu_1 \le 0$, which is a natural boundary.

(2) $\Phi(\mu^*) = (\Phi(\mu))^*$. (A5)

(3) For real $\lambda > 0$,

$$\tfrac{1}{2}[\Phi(i\lambda) + \Phi(-i\lambda)] = \tfrac{1}{2}\lambda + \sum_{1}^{\infty} n^{-1}\,e^{-n\lambda}\,\tanh(n\lambda). \qquad (A6)$$

This should be compared with Eq. (3.13).

(4) For all μ except points on the real axis,

$$\Phi(\mu) - \Phi(-\mu) = \sum_{0}^{\infty}\frac{(-1)^n}{2n+1}\,\cot\left(\frac{\pi^2(2n+1)}{2\mu}\right) - i\pi. \qquad (A7)$$

Proof: The integrand in (A1) with $\phi_0 \equiv 0$ has simple poles at

$$x_0(n) = (n + \tfrac{1}{2})i, \quad n = 0, \pm 1, \cdots, \qquad (A8)$$

and logarithmic branch points at

$$x_1^{\pm}(n) = \pm i + n\pi i/\mu, \qquad (A9a)$$

$$x_2(n) = n\pi i/\mu, \quad n = 0, \pm 1, \cdots. \qquad (A9b)$$

As μ moves away from the real axis, the branch points move in the x plane. Evidently $\Phi(\mu)$ may be analytically continued to the entire μ plane, except the negative real μ axis; in that case, the contour of integration is pinched by the branch points against the singularities $x_0(n)$, for *all* rational values of μ.

Since $\Phi(\mu)$ is real analytic and real on the line segment $(\mu_2 = 0, 0 < \mu_1 < \pi)$, the Schwarz principle gives (A5), the second part of Theorem 1.

In order to derive (A6) and (A7) and prove that $(\mu_2 = 0, \mu_1 \le 0)$ is a natural boundary, $\Phi(\mu)$ may be rewritten, using the Parseval formula, as

$$\Phi(\mu) = \tfrac{1}{2}\int_{-\infty}^{\infty} \frac{dx}{x} \frac{\sinh\mu x, \sinh(\pi-\mu)x}{\cosh\mu x, \sinh\pi x} \tag{A10}$$

provided $0 < \mu_1 < \pi$. (This result may be extended to other strips, but this will not be needed here.)

In this case, the integrand has simple poles at

$$p_1(n) = (n+\tfrac{1}{2})\,\pi i/\mu, \quad n = 0, \pm 1, \cdots, \tag{A11}$$

$$p_0(n) = ni, \quad n = \pm 1, \pm 2, \cdots. \tag{A12}$$

As μ rotates, the poles $p_1(n)$ rotate synchronously and impinge upon the real axis when $\mu = i\lambda$. An elementary, but tedious, calculation shows that

$$\Phi(i\lambda) = \frac{\lambda}{2} + \sum_1^{\infty} n^{-1}\, e^{-n\lambda} \tanh(n\lambda) + i\sum_0^{\infty} \frac{(-1)^n\, e^{-\pi^2(n+1/2)/\lambda}}{(n+\tfrac{1}{2})\sinh[(\pi^2/\lambda)(n+\tfrac{1}{2})]}. \tag{A13}$$

Using (2) of Theorem 1, one readily obtains (A6) from (A13) and the result

$$\Phi(i\lambda) - \Phi(-i\lambda) = -i\pi + 4i\sum_0^{\infty} \frac{(-1)^n}{(2n+1)} \times \coth\left(\frac{\pi^2(n+\tfrac{1}{2})}{\lambda}\right). \tag{A14}$$

According to the identity theorem for analytic functions, the analytic continuation of $\Phi(\mu)$, whenever it exists, must satisfy the equation

$$\Phi(\mu) - \Phi(-\mu) = -i\pi + 2\sum_0^{\infty} \frac{(-1)^n}{2n+1} \cot\left(\frac{\pi^2(2n+1)}{2\mu}\right). \tag{A15}$$

The series above represents an analytic function in the finite μ plane except for the line $\mu_2 = 0$, upon which there are simple poles at the points μ_0, given by

$$\mu_0 = \pi(2r+1)/2s, \tag{A16}$$

where r and s are any integers. In order to prove that the real axis is a natural boundary, we have to consider the approach to $\mu_2 = 0$ along a line

$$\mu = \pi(2r+1)/2s + i\mu_2. \tag{A17}$$

This gives

$$\Phi(\mu) - \Phi(-\mu) = \frac{4\mu(-1)^r}{\mu_2\pi(2r+1)^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2} + G(\mu_2, \mu_0), \tag{A18}$$

where $G(\mu_2, \mu_0)$ can be bounded. The sum of the series is the Catalan constant, which is nonzero. The intercepts of the lines given by (A17) with the real axis form a dense set of points in $\mathcal{R}$. Thus the line $\{\mu_2 = 0, -\infty < \mu_1 \le 0\}$ is a natural boundary. This completes the proof of Theorem 1. The physical interpretation will be described later.

When $n > 1$, the motion of the singularities in the integration plane for $\Phi(\mu)$ is complicated by the explicit dependence of φ_0 on μ. Nevertheless, we shall be able to prove an analog of Theorem 1, although we shall be content with a more restricted domain of analyticity for $\Phi(\mu)$.

There are μ-dependent branch points in the integration plane at

$$x_2^{\pm}(n) = \pm\, i(1 - \phi_0/2\mu) + n\pi i/\mu \tag{A19a}$$

and

$$x_2^{\pm}(n) = \pm\, i\phi_0/2\mu + n\pi i/\mu, \quad n = 0, \pm 1, \cdots, \tag{A19b}$$

as μ varies the contour of integration pinches the stationary poles at

$$x_0(n) = (n+\tfrac{1}{2})i, \quad n = 0, \pm 1, \cdots. \tag{A20}$$

It is clear that the motion of the branch points has an epicyclic character which arises from the dependence of ϕ_0 on μ. It should also be noted that singular behavior of $\Phi(\mu)$ is given by the branch points of $\phi_0(\mu)$ at

$$\mu = i\,|K_1| + (2n+1)\pi, \quad n = 0, \pm 1, \cdots. \tag{A21}$$

For $K_1 > 0$, $\varphi_0(\mu)$ is analytic in a neighborhood of the real positive μ axis. Also $\varphi_0/2\mu$ is real for real μ, so that in that case the branch points $x_j^{\pm}(n)$ lie on the imaginary axis. Clearly there exists an $\epsilon > 0$ (for $K_1 > 0$) such that $\Phi(\mu)$ is analytic in the domain

$$D_r = \{\mu:\ \mu_1 > 0, -\epsilon < \mu_2 < \epsilon\}. \tag{A22}$$

On the principal branch of $\varphi_0(\mu)$, we have by Taylor's theorem at $\mu = 0$ that

$$\frac{\varphi_0}{2\mu} = \frac{1}{2}\frac{\eta-1}{\eta+1}\left(1 + \frac{\eta}{3(\eta+1)^2}\,\mu^2\right) + O(\mu^4). \tag{A23}$$

Thus the eccentric motion of the epicycle may be made arbitrarily small by confining μ to a small enough disc about $\mu = 0$. Evidently there exists a neighborhood D_0 of $\mu = 0$ for which the motion of $x_j^{\pm}(n)$ is essentially synchronous with μ. In this case, the analysis of Theorem 1 can be taken over directly to prove that $\Phi(\mu)$ is analytic for all μ in D_0, except the set of points $\{\mu:\ \mu_2 = 0, \mu_1 \le 0\} \cap D_0$, which is a natural boundary.

The function $\Phi(\mu)$ will now be evaluated for $\mu = i\lambda$, $\lambda > 0$. Using the Parseval transform, one obtains

$$\Phi(\mu) = \tfrac{1}{2}\int_{-\infty}^{\infty} \frac{dx}{x} \frac{\sinh(\pi-\mu)x\, \sinh(\mu-\varphi_0)x}{\cosh\mu x\, \sinh\pi x} \tag{A24}$$

for $0 \le \mu,\ 0 < \pi,\ \mu_2 \ne 0$. By employing the same argument as for Theorem 1 (only the residues of the poles are changed), one may find

$$\Phi(i\lambda) = \frac{\lambda-\theta_0}{2} + \sum_1^{\infty} \frac{e^{-n\lambda}}{n} \frac{\sinh(\lambda-\theta_0)n}{\cosh(n\lambda)} + 2i\sum_0^{\infty} \frac{(-1)^n}{2n+1} \frac{\cos[(\pi\theta_0/\lambda)(n+\tfrac{1}{2})]}{\sin[(\pi^2/\lambda)(n+\tfrac{1}{2})]}\, e^{-(\pi^2/\lambda)(n+1/2)}, \tag{A25}$$

where θ_0 is given by (A2) with $\mu = i\lambda$. By using the analyticity of $\varphi_0(\mu)$ in a neighborhood of $\mu = i\lambda$, it is clear that there exists a $\delta > 0$ and a $\gamma(\delta) > 0$ such that $\Phi(\mu)$ is analytic in the domain D_i defined by

$$D_i = \{\mu: -\gamma(\delta) < \mu_1 < \gamma(\delta),\ |\mu_2| > \delta\}. \quad \text{(A26)}$$

The number δ in the above definition may be chosen so that $D_i \cap D_0 \neq \phi$. Thus $\Phi(\mu)$ is analytic everywhere in the domain $T = D_i \cup D_0 \cup D_r$ except for the set $\{\mu: \mu_2 = 0, \mu_1 \leq 0\} \cap D_0$, which is a natural boundary. Since $\Phi(\mu)$ is real analytic for $\mu_2 = 0$, $\mu_1 > 0$, it follows that

$$\Phi(\mu) = (\Phi(\mu^*))^* \quad \text{(A27)}$$

for $\mu \in T$, by the Schwartz reflection principle. Thus we have established the following theorem:

Theorem 2: If the variable η satisfies $\eta > 1$, then for all such values we have the following.

(1) $\Phi(\mu)$ may be analytically continued to a sector S of the μ plane given by

$$-(\tfrac{1}{2}\pi + \delta) \leq \arg\mu \leq (\tfrac{1}{2}\pi + \delta), \quad \delta > 0.$$

There are singularities at the branch points of $\phi_0(\mu)$ given by

$$\mu_n = \pm i|K_1| + (2n+1)\pi, \quad n = 0, \pm 1, \cdots.$$

(2) $\Phi(\mu^*) = (\phi(\mu))^*$.

(3) For $\lambda > 0$,

$$\tfrac{1}{2}[\Phi(i\lambda) + \Phi(-i\lambda)] = \frac{\lambda - \theta_0}{2} + \sum_1^\infty \frac{e^{-n\lambda}}{n} \frac{\sinh(\lambda - \theta_0)n}{\cosh n\lambda}$$

For fixed $\eta \geq 1$, in order to investigate the nature of the singularity of $\Phi(\mu)$ at $\mu = 0$ and its thermodynamic consequences, we have to find an asymptotic expansion for $\Phi(\mu)$ valid near $\mu = 0$. This may be done along the lines laid down by Yang and Yang.[10] Equation (A24) may be rewritten as

$$\Phi(\mu) = \tfrac{1}{2} \int_{-\infty}^{\infty} \frac{dx}{x \sinh\pi x} G(\mu, x), \quad \text{(A28)}$$

where

$$G(\mu, x) = \frac{\sinh(\pi - \mu)x \sinh(\mu - \varphi_0)x}{\cosh\mu x}. \quad \text{(A29)}$$

We define the set S of points in the μ plane by the prescription

$$|\mu| \leq r, \quad -\delta_0 \leq \arg\mu \leq 0, \quad \text{(A30a)}$$

where

$$\delta_0 = \pi - \epsilon, \quad \epsilon > 0. \quad \text{(A30b)}$$

Let the straight line P be given by

$$x = te^{i(\pi - \epsilon)/2}, \quad -\alpha < t < \infty. \quad \text{(A31)}$$

For $\mu \in S$, P is always free of poles of $G(\mu, x)$; consequently the integration path may be deformed to P. Along P, however, all the derivatives with respect to μ of $G(\mu, x)$ are bounded for $\mu \in S$ and so we have the following.

(1) $G(\mu, x) = \sum_0^n c_j(x)\, \mu^j + g_n(x)\, \mu^{n+1}$, (A32)

where $g_n(x) \leq M_n$ for all $x \in P$.

(2) The functions $g_n(x)$ and $c_j(x)$ and even, with

$$g_n(0) = c_j(0) = 0. \quad \text{(A33)}$$

It follows that

$$\Phi(\mu) = \sum_0^n d_j\mu^j + O(\mu^{n+1}), \quad \text{(A34a)}$$

where

$$\alpha_j = \tfrac{1}{2} \int_{-\infty}^{\infty} \frac{c_j(x)\, dx}{x \sinh\pi x}. \quad \text{(A34b)}$$

The d_j must grow sufficiently fast to make the radius of convergence of (A34a) zero. The differential coefficients of $\Phi(\mu)$ with respect to μ and η at the point $(\mu = 0, \eta = \eta_0)$ are evidently obtained by termwise differentiation of (A34a). The coefficients d_j may be obtained by rewriting

$$\Phi(\mu) = J_1(\mu) + J_2(\mu), \quad \text{(A35a)}$$

where

$$J_1(\mu) = \tfrac{1}{2} \int_0^\infty \frac{dx}{x} \operatorname{sech}(\mu x)\, (e^{-\varphi_0 x} - e^{-(2\mu - \varphi_0)x})$$

$$= \log\left(\frac{\Gamma(1 + s/4)\, \Gamma(\tfrac{1}{2} - s/4)}{\Gamma(1 - s/4)\, \Gamma(\tfrac{1}{2} + s/4)}\right) \quad \text{(A35b)}$$

with

$$s = 1 - \varphi_0/\mu. \quad \text{(A35c)}$$

The other integral $J_2(\mu)$ is given by

$$J_2(\mu) = \int_0^\infty \frac{dx}{x} \frac{e^{-\pi x}}{\cosh(\mu x) \sinh\pi x} \times \sinh\varphi_0 x \sinh(\mu - \varphi_0)x \quad \text{(A35d)}$$

which may be rewritten as

$$J_2(\mu) = \int_0^\infty \frac{dy}{y} \left[\exp\left(\frac{2\pi y}{\mu}\right) - 1\right]^{-1} \times \frac{\cosh(1 - s)y - \cosh(1 + s)y}{\cosh y}. \quad \text{(A35e)}$$

The generating function

$$\frac{e^{(2\lambda - 1)x}}{\cosh x} = \sum_0^\infty E_n(\lambda) \frac{(2x)^n}{n!}, \quad |x| < \pi/2, \quad \text{(A36)}$$

for the Euler polynomials, and the formula

$$E_n(1 - x) = (-1)^n E_n(x) \quad \text{(A37)}$$

give the formula

$$J_2(\mu) = \int_0^\infty \frac{dy}{y} \left[\exp\left(\frac{2\pi y}{\mu}\right) - 1\right]^{-1} \sum_1^\infty \frac{y^{2n}}{(2n)!} \times \left[E_{2n}\left(\frac{s}{2}\right) - E_{2n}\left(\frac{-s}{2}\right)\right]. \quad \text{(A38)}$$

By using the standard integral

$$\int_0^\infty \frac{dy}{y} \left[\exp\left(\frac{2\pi y}{\mu}\right) - 1\right]^{-1} y^{2n} = \frac{2^{2n}(-1)^{n+1}}{4n} \mu^{2n} B_{2n}, \quad \text{(A39)}$$

one readily finds that

$$J_2(\mu) = \sum_1^\infty \frac{2^{2n}}{(2n)!} \left[E_{2n}\left(\frac{-s}{2}\right) - E_{2n}\left(\frac{s}{2}\right)\right] B_{2n} \frac{(i\mu)^{2n}}{4n}. \quad \text{(A40)}$$

Thus $\Phi(\mu)$ has the asymptotic expansion

$$\Phi(\mu) = \log \frac{\Gamma(1+s/4)\,\Gamma(\frac{1}{2}-s/4)}{\Gamma(1-s/4)\,\Gamma(\frac{1}{2}+s/4)} + \sum_1^\infty \frac{2^{2n}}{(2n)!}\left[E_{2n}\left(\frac{-s}{2}\right) - E_{2n}\left(\frac{s}{2}\right)\right] B_{2n}\,\frac{(i\mu)^{2n}}{4n}, \tag{A41}$$

valid for $\mu \in S$, defined by (A30).

The crucial point is that only even powers of μ appears in (A41), and $\Phi(\mu)$ belongs to the class C^∞ under differentiation with respect to μ^2 at $\mu = 0$ along any radial line in S. By the implicit function theorem, μ^2 is an analytic function of Δ in a neighborhood of $\Delta = -1$. Thus one concludes that, even though $\Phi(\mu)$ is not analytic at $\mu = 0$, nevertheless all temperature derivatives of $z(0)$ exist at $T = T_0$ (corresponding to $\Delta = -1$) and are continuous there. We see that the F model results are prototypical for any $\Delta = -1$ transition point; such transition points are of infinite order in the Ehrenfest scheme.

APPENDIX B

Consider the function

$$I(\alpha,\beta,\gamma) = \int_0^\infty \operatorname{sech}(\alpha x)\ln\left(\frac{\cosh x - \cos\beta}{\cosh x - \cos\gamma}\right)dx. \tag{B1}$$

Let the function $F(\beta,y)$ be defined by the integral

$$F(\beta,y) = \tfrac{1}{2}\int_{-\infty}^{\infty} \frac{e^{ixy}}{\cosh x - \cos\beta}\,dx. \tag{B2}$$

Then, for $0 < \mathrm{Re}\beta \le \pi$, we have by contour integration

$$F(\beta,y) = \frac{\pi}{\sin\beta}\,\frac{\sinh[(\pi-\beta)y]}{\sinh(\pi y)}. \tag{B3}$$

These results may be extended to other strips in the β plane by use of the relation

$$F(\beta,y) = F(2k\pi \pm \beta, y) \tag{B4}$$

although $F(\beta,y)$ is not defined for $\mathrm{Re}\beta = 2n\pi$.

The Fourier cosine transform of $\ln[(\cosh x - \cos\beta)/(\cosh x - \cos\gamma)]$ is readily obtained from this function. Since $\sin\beta F(\beta,y)$ is continuous for $0 \le \beta \le 2\pi$, we may integrate it with respect to β. Furthermore, the infinite integrand in (B2) is uniformly convergent with respect to β in $0 < \beta < 2\pi$ so that the order of integration may be reversed in that interval giving

$$\int_0^\infty dx\,\cos xy\,\ln\left(\frac{\cosh x - \cos\beta}{\cosh x - \cos\gamma}\right) = \frac{2\pi}{y}\,\mathrm{csch}(\pi y)\sinh[(\pi\tfrac{1}{2}(\gamma+\beta))y]\sinh[\tfrac{1}{2}(\beta-\gamma)y] = \frac{\pi}{y}\{e^{-\gamma y} - e^{-\beta y} + 2e^{-\pi y}\,\mathrm{csch}(\pi y)\sinh(\tfrac{1}{2}(\gamma+\beta)y) \times \sinh[\tfrac{1}{2}(\gamma-\beta)y]\}. \tag{B5}$$

The Fourier cosine transform of $\operatorname{sech}(\alpha x)$ is

$$\int_0^\infty \cos(xy)\operatorname{sech}(\alpha x)\,dx = (\pi/2\alpha)\operatorname{sech}(\pi y/2\alpha). \tag{B6}$$

Application of the Parseval theorem to (B1) gives

$$I(\alpha,\beta,\gamma) = \frac{\pi}{\alpha}\int_0^\infty \frac{dy}{y}\operatorname{sech}\left(\frac{\pi y}{2\alpha}\right)\{2e^{-\pi\gamma}\,\mathrm{csch}(\pi y) \times \sinh[\tfrac{1}{2}(\gamma+\beta)y]\sinh[\tfrac{1}{2}(\gamma-\beta)y] + e^{-\gamma y} - e^{-\beta y}\} \tag{B7}$$

for $0 < \mathrm{Re}(\beta,\gamma) < 2\pi$. The extension of this to other ranges of β and γ is achieved by using the relation

$$I(\alpha,\beta,\gamma) = I(\pm\alpha + 2k\pi i, \pm\beta + 2l\pi, \pm\gamma + 2m\pi). \tag{B8}$$

The evaluation of the free energy for KDP and IKDP will now be considered. By using the Laplace transform

$$\int_0^\infty e^{-pt}\left(\frac{1-\operatorname{sech} t}{t}\right)dt = 2\ln\frac{2\Gamma(\frac{1}{4}p+\frac{3}{4})}{p^{1/2}\Gamma(\frac{1}{4}p+\frac{1}{4})}. \tag{B9}$$

it follows that

$$\int_0^\infty \frac{dy}{y}\operatorname{sech}\left(\frac{\pi y}{2\alpha}\right)(e^{-\gamma y} - e^{-\beta y}) = 2\ln\frac{\Gamma(\beta\alpha/2\pi+\frac{3}{4})\Gamma(\gamma\alpha/2\pi+\frac{1}{4})}{\Gamma(\beta\alpha/2\pi+\frac{1}{4})\Gamma(\gamma\alpha/2\pi+\frac{3}{4})}. \tag{B10}$$

I. KDP

From (3.3)

$$-\beta\mathfrak{F}_{\mathrm{KDP}} = (1/4\mu)\,I(\pi/2\mu, \mu, 3\mu - 2\pi), \tag{B11}$$

where $2\pi/3 \le \mu \le \pi$. The remaining integral in (B7) may be evaluated by appealing to the table of Laplace transforms in Ref. 16. Thus

$$-\beta\mathfrak{F}_{\mathrm{KDP}} = \ln|(2\mu/\pi)\cot(\pi^2/2\mu)\csc\mu|. \tag{B12}$$

II. IKDP

In this case we have

$$-\beta\mathfrak{F}_{\mathrm{IKDP}} = -K + (1/4\mu)[I(\pi/2\mu, 5\mu - 2\pi, \mu) + I(\pi/2\mu, \mu, 3\mu)] \tag{B13}$$

with $\pi/2 \le \mu \le 2\pi/3$. This gives

$$-\beta\mathfrak{F}_{\mathrm{IKDP}} = \ln|(2\mu/\pi)\cot(\pi^2/2\mu)\csc\mu|. \tag{B14}$$

This same formula therefore holds for KDP and IKDP, the values of μ lying in different ranges.

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Part X

Ising and Dimer Models

Two-Dimensional Ising Model as a Soluble Problem of Many Fermions

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I. INTRODUCTION

The two-dimensional Ising model for a system of interacting spins (or for the ordering of an AB alloy) on a square lattice is one of the very few nontrivial many-body problems that is exactly soluble and shows a phase transition. Although the exact solution in the absence of an external magnetic field was first given almost twenty years ago in a famous paper by Onsager[1] using the theory of Lie algebras, the flow of papers on both approximate and exact methods has remained strong to this day.[2] One reason for this has been the interest in testing approximate methods on an exactly soluble problem. A second reason, no doubt, has been the considerable formidability of the Onsager method. The simplification achieved by Bruria Kaufman[3] using the theory of spinor representations has diminished, but not removed, the reputation of the Onsager approach for incomprehensibility, while the subsequent application of this method by Yang[4] to the calculation of the spontaneous magnetization has, if anything, helped to restore this reputation.

The principal alternative line to these algebraic methods has been to reduce the problem to one of counting polygons on a lattice—the so-called combinatorial method.[5] The first important steps in this direction were achieved by Kac and Ward[6] and by Potts and Ward,[7] although a rigorous combinatorial solution has only recently been given by Hurst and Green[8] and Kasteleyn,[9] the spontaneous magnetization being calculated by Montroll, Potts, and Ward.[10] The combinatorial method, despite its reliance on certain ingenious topological tricks and on relatively unfamiliar entities call Pfaffians, certainly seems simple in contrast to the earlier algebraic methods and may have seemed destined to displace the former as the classical method of solution of this famous problem.

The present paper tries to restore the balance by presenting the algebraic approach in a way that is both very simple and intimately connected with the problem of a soluble many-fermion system. Except for one or two crucial steps, the approach is straightforward and requires no more than a knowledge of the elementary properties of spin $\frac{1}{2}$ and the second quantization formalism for fermions. Certain similarities to the method of linear canonical transformations employed by Bogolubov[11] and Valatin[12] in the theory of superconductivity is obvious but familiarity with these methods is not necessary to understand the present approach. It becomes apparent that the two-dimensional Ising model, rather than being entirely different from the trivially soluble many-body problems, reduces in some ways to one of them, being just the diagonization of a quadratic form.

In Sec. II the transfer matrix formalism, which is the heart of the algebraic approach, is rederived in the conventional way and also in a way that to us seems more natural. In Sec. III the transfer matrix is diagonalized for a lattice wrapped on a torus, using the formalism of second quantization for fermions. In Sec. IV, the two-spin correlation function in an infinite lattice is investigated and the different approaches of previous authors are reconciled. In Sec. V, various definitions of the spontaneous magnetization are contrasted and one of these is used to derive previous results. The rigorous steps heretofore omitted in the

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calculation of the spontaneous magnetization are all supplied.

The paper ends with a skeleton outline of the various steps required in the demonstration. The reader may find it advantageous at this time to examine this outline, given in Sec. VI, and also to return to it from time to time while following the detailed development of Secs. II–V. He should also avail himself of at least one of the Refs. 1 and 2 for collateral reading, discussion of the specific heat curve, etc.

II. FORMULATION OF PROBLEM

A. Introduction

We consider a set of spin $\frac{1}{2}$'s arranged on a square lattice of M columns and N rows, interacting only with nearest neighbors and with a magnetic field $\mathfrak{H}$. (We, ultimately, let M and N tend to infinity together, i.e., with M/N a fixed ratio, and denote this limit by $\lim_{M,N\to\infty}$.) Let the Hamiltonian be

$$\mathcal{H}(\sigma_{11},\cdots,\sigma_{NM})=-\mathfrak{H}\sum\sigma_{nm}-J_1\sum\sigma_{nm}\sigma_{n+1,m}-J_2\sum\sigma_{nm}\sigma_{n,m+1}. \quad (2.1)$$

(nm) refers to the site in the nth row and mth column, J_1 and J_2 are, respectively, the bond strengths within the columns and within the rows, and we have set the Bohr magneton equal to unity. Each σ_{nm} is a classical variable taking on the values ±1; or equivalently, the σ_{nm} are operators having eigenvalues ±1 (e.g., $\sigma^z{}_{nm}=2S^z{}_{nm}$, where $S^z{}_{nm}$ is the x component of the nmth spin operator). Because the interaction strengths of the horizontal and vertical bonds in the lattice are not assumed the same, one might call $\mathcal{H}$ the Hamiltonian for a "rectangular" Ising lattice. For boundary conditions, we can assume either that the lattice is wrapped on a torus, so that $\sigma_{n,M+1}=\sigma_{n1}$, $\sigma_{N+1,m}=\sigma_{1m}$, and the sums extend to N and M, or we can assume that the lattice has free ends, in which case the sums extend only to $N-1$ and $M-1$. Each boundary condition has its advantages and disadvantages, as we shall see.

The free energy F per spin of the system is obtained from the partition function either by

$$\exp(-\beta FNM)=Z\equiv\sum_{\sigma_{11}=\pm1}\cdots\sum_{\sigma_{NM}=\pm1}\exp[-\beta\mathcal{H}(\sigma_{11},\cdots,\sigma_{NM})] \quad (2.2)$$

if the σ's are considered as classical variables, or by

$$\exp(-\beta FNM)=Z\equiv \mathrm{tr}_{\sigma^z{}_{11}}\cdots\mathrm{tr}_{\sigma^z{}_{NM}}\times\exp[-\beta\mathcal{H}(\sigma^z{}_{11},\cdots,\sigma^z{}_{NM})] \quad (2.2')$$

if the σ's are considered as twice the x components of spin operators.

Also of interest, in calculating the spontaneous magnetization, is a two-spin correlation function defined by

$$\langle\sigma^z{}_{n'm'}\sigma^z{}_{nm}\rangle=Z^{-1}\,\mathrm{tr}_{\sigma^z{}_{11}\cdots\sigma^z{}_{NM}}\sigma^z{}_{n'm'}\sigma^z{}_{nm}\times\exp[-\beta\mathcal{H}(\sigma^z{}_{11}\cdots\sigma^z{}_{NM})]. \quad (2.3)$$

Averages of other functions of the spins can be defined in a similar way.

The problem under consideration is a special case of the more general Ising problem in any number of dimensions defined by the Hamiltonian

$$\mathcal{H}=-\tfrac{1}{2}\sum_{ij}J(\mathbf{R}_i-\mathbf{R}_j)\sigma_{\mathbf{R}_i}\sigma_{\mathbf{R}_j}-\mathfrak{H}\sum_i\sigma_{\mathbf{R}_i}.$$

If the $\sigma_{\mathbf{R}}$ variables were continuous, rather than confined to the two values ±1, then even this Hamiltonian and the corresponding free energy would be trivially soluble by simply introducing running wave variables

$$\sigma_{\mathbf{q}}=(NM)^{-\frac{1}{2}}\sum_i\exp(i\mathbf{q}\cdot\mathbf{R}_i)\sigma_{\mathbf{R}_i}$$

in terms of which the Hamiltonian is immediately diagonalized to

$$\mathcal{H}=-\sum\epsilon_{\mathbf{q}}\sigma^*{}_{\mathbf{q}}\sigma_{\mathbf{q}}-\mathfrak{H}\sigma_0(NM)^{\frac{1}{2}}$$

with

$$\epsilon_{\mathbf{q}}=(2NM)^{-1}\sum J(\mathbf{R}_i-\mathbf{R}_j)\exp[i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)].$$

Unfortunately this running-wave transformation is not available for the actual Ising problem because the constraint $\sigma_{\mathbf{R}_i}=\pm1$ leads to extremely complex conditions on the transformed variables, $\sigma_{\mathbf{q}}$. The spherical model, in which this constraint is replaced by the much weaker constraint $\sum\sigma_{\mathbf{R}}{}^2=NM$, is solvable by introducing running waves, but it is neither an exact solution to the Ising problem nor even a reliable guide. As we see, running waves *can* be introduced into the Ising problem to take advantage of the translational degeneracy, but only after some subtle algebraic preparations which are only possible with nearest neighbor interactions in one or two dimensions. This, then, is the reason for restricting the Hamiltonian to the special form of (2.1).

B. Conventional Derivation of the Transfer Matrix

The fundamental observation on which the algebraic approach is based is that the partition function is the trace of the Nth power of a certain matrix, which we call the *transfer matrix*. In this section we recall the conventional derivation of this result,[13] which has the advantage of algebraic simplicity. In the next section

[13] See the review of Newell and Montroll, Ref. 2. This and related methods were originally discovered by E. W. Montroll, J. Chem. Phys. 9, 706 (1941); H. A. Kramers and G. H. Wannier, Phys. Rev. 60, 252 (1941); E. N. Lassettre and J. P. Howe, J. Chem. Phys. 9, 747 (1941); and R. Kubo, Busseiron Kenkyu 1, 1943.

we give an alternate derivation which, although not so simple in its details, is perhaps more natural and straightforward (in the sense that it is formulated in the language of density matrices and reduced density matrices familiar from the many-body problem).

Consider first a one-dimensional cyclic lattice, so that

$$Z=\sum_{\sigma_1,\cdots,\sigma_N}\exp\left(K_1\Sigma\sigma_n\sigma_{n+1}\right)\exp\left(H\Sigma\sigma_n\right), \quad (2.4)$$

where

$$K_1=\beta J_1 \quad \text{and} \quad H=\beta\mathfrak{H}. \quad (2.5)$$

To bring out the fact that the multiple sum is a matrix product, we rewrite (2.4):

$$Z=\sum_{\sigma_1\sigma_1'\cdots\sigma_N\sigma_N'}[\exp\left(K_1\sigma_1'\sigma_2\right)][\exp\left(H\sigma_2\right)\delta_{\sigma_2\sigma_2'}]\cdots \times[\exp\left(K_1\sigma_N'\sigma_1\right)][\exp\left(H\sigma_1\right)\delta_{\sigma_1\sigma_1'}]. \quad (2.6)$$

If one defines the two 2×2, matrices

$$(\mathbf{V}_1)_{\sigma_i\sigma_j}=\exp\left(K_1\sigma_i\sigma_j\right)$$

or

$$\mathbf{V}_1=\begin{array}{c|cc} & \sigma_j=+1 & \sigma_j=-1 \\ \hline \sigma_i=+1 & e^{K_1} & e^{-K_1} \\ \sigma_i=-1 & e^{-K_1} & e^{K_1} \end{array} \quad (2.7a)$$

and

$$(\mathbf{V}_2)_{\sigma_i\sigma_j}=\exp\left(H\sigma_i\right)\delta_{\sigma_i\sigma_j}$$

or

$$\mathbf{V}_2=\begin{array}{c|cc} & \sigma_j=+1 & \sigma_j=-1 \\ \hline \sigma_i=+1 & e^{H} & 0 \\ \sigma_i=-1 & 0 & e^{-H} \end{array}, \quad (2.7b)$$

then Z is obviously the trace of a matrix product:

$$Z=\operatorname{tr}\mathbf{V}_1\mathbf{V}_2\cdots\mathbf{V}_1\mathbf{V}_2=\operatorname{tr}\left(\mathbf{V}_1\mathbf{V}_2\right)^N. \quad (2.8)$$

From the invariance of the trace under cyclic permutations of factors, Z can also be written as

$$Z=\operatorname{tr}\left(\mathbf{V}_2^{\frac{1}{2}}\mathbf{V}_1\mathbf{V}_2^{\frac{1}{2}}\right)^N\equiv\operatorname{tr}\mathbf{V}^N \quad (2.9)$$

or as

$$Z=\operatorname{tr}\left(\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}\right)\equiv\operatorname{tr}\mathbf{V}'^N, \quad (2.9')$$

which have the advantage that $\mathbf{V}$ and $\mathbf{V}'$ are symmetric. We call $\mathbf{V}$ (or $\mathbf{V}'$) the *transfer matrix*.[14]

[14] The transfer matrix, formulated first in general terms by Montroll[12] and also at the same time by Lasettre and Howe,[13] by Kramers and Wannier,[12] and perhaps others, is a powerful operational technique for describing the propagation down an arbitrary line of physical elements. It can be useful even when there is no translational invariance, e.g., the one-dimensional chain of vibrating atoms with random masses analyzed by Schmidt.[15] The one-dimensional Ising model with random bond strengths can also be solved, although the two-dimensional Ising model with some kind of randomness in the bonds has not yet been solved.

[15] H. Schmidt, Phys. Rev. 105, 425 (1957).

If Λ_1 and Λ_2 are the larger and smaller eigenvalues of $\mathbf{V}$, respectively, then

$$Z=\Lambda_1^N+\Lambda_2^N=\Lambda_1^N[1+(\Lambda_2/\Lambda_1)^N]. \quad (2.10)$$

As $N\to\infty$, the free energy per spin is

$$F=-kT\log\Lambda_1, \quad (2.11)$$

the contribution of Λ_2^N being negligible. Thus *finding the free energy reduces to determining the largest eigenvalue of the transfer matrix.*

The matrices $\mathbf{V}_1$, $\mathbf{V}_2$, and $\mathbf{V}$, being 2×2 matrices, can be written in terms of the four Pauli matrices, which we call $\mathbf{1}$, τ^x, τ^y and τ^z (we use τ's rather than σ's to avoid confusion with the σ variables already introduced):

$$\mathbf{V}_1=e^{K_1}\mathbf{1}+e^{-K_1}\tau^x=e^{K_1}(\mathbf{1}+e^{-2K_1}\tau^x), \quad (2.12a)$$

$$\mathbf{V}_2=\mathbf{1}\cosh H+\tau^z\sinh H. \quad (2.12b)$$

It is convenient for the generalization to two dimensions to express $\mathbf{V}_1$ and $\mathbf{V}_2$ as exponentials of the Pauli matrices. For this purpose recall the property of the τ^i, $(i=x,\ y,\ z)$, that because $(\tau^i)^2=1$,

$$\exp\left(a\tau^i\right)=\mathbf{1}\cosh a+\tau^i\sinh a=(\cosh a)\left(\mathbf{1}+\tau^i\tanh a\right) \quad (2.13)$$

for any number a. Then $\mathbf{V}_2$ becomes immediately

$$\mathbf{V}_2=\exp\left(H\tau^z\right). \quad (2.14)$$

To simplify $\mathbf{V}_1$ with (2.13), we define K_1^* by[16]

$$\tanh K_1^*\equiv e^{-2K_1}, \quad (2.15a)$$

whereupon

$$\mathbf{V}_1=(2\sinh 2K_1)^{\frac{1}{2}}\exp\left(K_1^*\tau^x\right). \quad (2.16)$$

We have used the simple identities

$$\tanh K_1\equiv e^{-2K_1^*} \quad \text{and} \quad \sinh 2K_1\sinh 2K_1^*\equiv 1 \quad (2.15b)$$

implied by (2.15a).

The generalization to the two-dimensional problem follows immediately. Instead of summing over the two orientations of each spin, we must sum over the 2^M configurations of each row. The matrix $\mathbf{V}_2$ is still diagonal and can be written

$$\mathbf{V}_2=\exp\left(K_2\sum\tau_m^z\tau_{m+1}^z+H\sum\tau_m^z\right).$$

Because the two sums in the exponent commute and represent different physical mechanisms, it is customary to replace $\mathbf{V}_2$ in (2.8) or (2.9) by $\mathbf{V}_2\mathbf{V}_3$, where

$$\mathbf{V}_2=\exp\left(K_2\sum\tau_m^z\tau_{m+1}^z\right) \quad \text{and} \quad \mathbf{V}_3=\exp\left(H\sum\tau_m^z\right). \quad (2.16)$$

[16] K_1^* should not be confused with "complex conjugate of K_1", which is real of course.

The matrix $\mathbf{V}_1$ is similarly generalized from the one-dimensional case:

$$\mathbf{V}_1=(2\sinh 2K_1)^{M/2}\exp\,(K_1^*\textstyle\sum\tau^x_m). \quad (2.17)$$

Now the matrices τ^z_m and τ^x_m are $2^M\times 2^M$ matrices defined as direct products[17]

$$\tau^z_m=\mathbf{1}\times\cdots\times\mathbf{1}\times\tau^z\times\mathbf{1}\times\cdots\times\mathbf{1} \quad (2.18a)$$

$$\tau^x_m=\mathbf{1}\times\cdots\times\mathbf{1}\times\tau^x\times\mathbf{1}\times\cdots\times\mathbf{1} \quad (2.18b)$$

and

$$Z=\mathrm{tr}[(\mathbf{V}_2\mathbf{V}_3)^{\frac{1}{2}}\mathbf{V}_1(\mathbf{V}_2\mathbf{V}_3)^{\frac{1}{2}}]^N=\mathrm{tr}\,\mathbf{V}^N. \quad (2.19)$$

This is the conventional formulation in terms of the transfer matrix. Although very direct, it introduces the matrices τ^z_m and τ^x_m as an artificial device, distinct from the operators σ^z_{nm}, σ^x_{nm}.

C. Alternate Derivation of the Transfer Matrix

Because the τ matrices are isomorphic to the σ operators of a single row, it is possible to derive the transfer matrix formalism without introducing the τ's at all. In this section we present such a derivation, which is in some ways more natural than that of the preceding section, although the results are the same.

Consider a lattice of N rows and M columns, *not* on a torus (although perhaps on a cylinder, so that each row is cyclic). If N is large, it is physically reasonable to expect that the probability of a given configuration of the last row, when one averages over all configurations of the other $N-1$ rows, should be asymptotically independent of N. This suggests trying to find a recursion relation between the probability distribution of configurations of the final row in lattices of N and $N+1$ rows.

To derive such a recursion relation we consider the *density operator* for $N+1$ rows,

$$\rho_N(\Sigma_0,\Sigma_1,\cdots,\Sigma_N)=\exp\,[\sum_1^N(\mathcal{K}_n+\mathcal{K}_n^{(1)}+\mathcal{K}_n^{(2)})]\rho_0(\Sigma_0), \quad (2.20)$$

where

$$\mathcal{K}_n=H\sum_m\sigma^x_{nm},$$

$$\mathcal{K}_n^{(1)}=K_1\sum_m\sigma^x_{n-1,m}\sigma^x_{nm},$$

$$\mathcal{K}_n^{(2)}=K_2\sum_m\sigma^x_{nm}\sigma^x_{n,m+1}, \quad (2.21)$$

[17] If one has two vector spaces with sets of basis vectors denoted, respectively, by $|\alpha\rangle$ and $|a\rangle$ and operators $\mathfrak{A}$ and $\mathbf{A}$ defined, respectively, in these vector spaces, then the direct product $\mathfrak{A}\times\mathbf{A}$ is defined in the vector space with basis vectors denoted by $|\alpha a\rangle$ by the matrix elements

$$\langle\beta b|\mathfrak{A}\times\mathbf{A}|\alpha a\rangle=\langle\beta|\mathfrak{A}|\alpha\rangle\langle b|\mathbf{A}|a\rangle.$$

Thus the operator $\mathfrak{A}$ can be considered in the larger space as the direct product $\mathfrak{A}\times\mathbf{1}$, etc., where $\mathbf{1}$ is the unit operator in the space of the $|a\rangle$'s. The generalization to direct products of more than two operators is obvious.

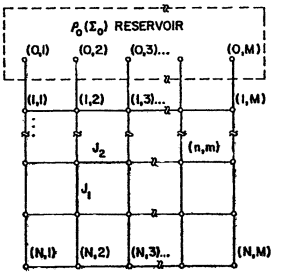

FIG. 1. Two-dimensional Ising lattice of $N+1$ rows and M columns, in which zeroth row is connected to a special reservoir.

and Σ_n is a shorthand symbol for $(\sigma^x_{n1},\cdots,\sigma^x_{nM})$. We assume that the x components, rather than the more conventional z components, of the spins interact with each other and with the magnetic field, to simplify some of the algebra. The density operator for the zeroth row, $\rho_0(\Sigma_0)$, is as yet arbitrary and allows us to see the effect of the conditions at one edge of the lattice on the bulk properties. The model described by (2.20) is shown pictorially in Fig. 1.

The *reduced density operator* for the last row is

$$\rho_N(\Sigma_N)\equiv\mathrm{tr}_{\Sigma_0,\Sigma_1,\ldots,\Sigma_{N-1}}\rho_N(\Sigma_0,\Sigma_1,\cdots,\Sigma_N). \quad (2.22)$$

This operator can be expressed in terms of the reduced-density operator for the last row in an N row system by the obvious recursion relation

$$\rho_N(\Sigma_N)=\exp\,(\mathcal{K}_N+\mathcal{K}_N^{(2)})\,\mathrm{tr}_{\Sigma_{N-1}}\times\exp\,(\mathcal{K}_N^{(1)})\rho_{N-1}(\Sigma_{N-1}). \quad (2.23)$$

The trace on the right can be considerably simplified if we observe that, because $(\sigma^x_m)^{2r}=1$ and $(\sigma^x_m)^{2r+1}=\sigma^x_m$, one can think of $\rho_{N-1}(\Sigma_{N-1})$ as being expanded in a canonical form:

$$\rho_{N-1}(\Sigma_{N-1})=a^{(0)}+\sum_{m_1}a^{(1)}{}_{m_1}\sigma^x_{m_1}+\sum_{m_1\le m_2}a^{(2)}{}_{m_1m_2}\sigma^x_{m_1}\sigma^x_{m_2}+\cdots, \quad (2.24)$$

where we have designated $\sigma^x_{N-1,m}$ by σ^x_m, etc. There are

$$\binom{M}{0}+\binom{M}{1}+\cdots+\binom{M}{M-1}=2^M$$

coefficients in the series (2.24), corresponding to the 2^M configurations of the $(N-1)$st row. Consider the contribution to the trace in (2.23) of a typical term in $\rho_{N-1}(\Sigma_{N-1})$:

$$\mathrm{tr}_\Sigma\exp\,(\mathcal{K}_N^{(1)})\sigma^x_{m_1}\cdots\sigma^x_{m_r}=\mathrm{tr}_\Sigma\prod_m\exp\,(K_1\sigma^x_m{}'\sigma^x_m)\sigma^x_{m_1}\cdots\sigma^x_{m_r} \quad (2.25)$$

where we also designate σ^x_{Nm} by $\sigma^x_m{}'$. Now

$$\mathrm{tr}_{\sigma^x_m} \exp\,(K_1\sigma^x_m{}'\sigma^x_m) = 2\cosh\,(K_1\sigma^x_m{}') = 2\cosh K_1 \tag{2.26a}$$

and

$$\mathrm{tr}_{\sigma^x_m} \exp(K_1\sigma^x_m{}'\sigma^x_m)\sigma^x_m = 2\sinh\,(K_1\sigma^x_m{}') = 2\sigma^x_m{}'\sinh K_1. \tag{2.26b}$$

Thus

$$\mathrm{tr}_\Sigma \exp(\mathcal{K}_N{}^{(1)}\sigma^x_{m_1}\cdots\sigma^x_{m_r}) = (2\cosh K_1)^M(\tanh K_1)^r\sigma^x_{m_1}{}'\cdots\sigma^x_{m_r}{}' \tag{2.27}$$

and, if $\rho_{N-1}(\sigma^x_1, \cdots, \sigma^x_M)$ is considered to be written in its canonical form, then

$$\mathrm{tr}_{\Sigma_{N-1}} \exp(\mathcal{K}_N{}^{(1)})\rho_{N-1}(\sigma^x_{N-1,1}, \cdots, \sigma^x_{N-1,M}) = (2\cosh K_1)^M\rho_{N-1}(\sigma^x_{N1}\tanh K_1, \cdots, \sigma^x_{NM}\tanh K_1). \tag{2.28}$$

We now try to find an operator $\mathcal{O}$ having the property that

$$(2\cosh K_1)^M\rho_{N-1}(\sigma^x_{N1}\tanh K_1, \cdots, \sigma^x_{NM}\tanh K_1) = \mathcal{O}\rho_{N-1}(\sigma^x_{N1}, \cdots, \sigma^x_{NM}), \tag{2.29}$$

because we would then have the simple recursion relation

$$\rho_N(\Sigma_N) = \exp\,(\mathcal{K}_N + \mathcal{K}^{(2)}_N)\,\mathcal{O}\rho_{N-1}(\Sigma_N). \tag{2.30}$$

If $\mathcal{O}$ exists it must clearly have the form

$$(2\cosh K_1)^M(\tanh K_1)^{\mathfrak{N}},$$

where $\mathfrak{N}$ is an operator that counts the number of σ^x's in any term of the canonical expansion. In particular, for the zeroth-order term, we would require that $\mathfrak{N}\cdot 1 = 0$ or $\mathfrak{N} = 0$, which does not meet the requirements for other terms of the expansion. Thus there exists no operator $\mathcal{O}$ in the algebra of the σ^x's that makes (2.29) an operator identity. It is possible, however, to satisfy (2.29) when both sides are applied to a particular state. It is especially convenient (and sufficient to obtain tr $\rho_N(\Sigma_N)$, as we shall see) to take as that state the state with all spins down, which we call the "vacuum" and denote by $|\,0\rangle$:

$$\sigma^-_{Nm}\,|\,0\rangle = 0, \quad \text{all } m. \tag{2.31}$$

Then

$$\sigma^x_{Nm}\,|\,0\rangle = \sigma^+_{Nm}\,|\,0\rangle, \tag{2.32}$$

so that the operator $\mathfrak{N}$, which must count the number of distinct σ^x's present in a product, is just the operator that counts the number of up spins,

$$\mathfrak{N} = \sum_m \sigma^+_{Nm}\sigma^-_{Nm}. \tag{2.33}$$

In this way, from (2.28) we obtain the recursion relation

$$\rho_N(\Sigma_N)\,|\,0\rangle = \exp\,(\mathcal{K}_N + \mathcal{K}_N{}^{(2)})\,(2\cosh K_1)^M \times (\tanh K_1)^{\Sigma\sigma^+_m\sigma^-_m}\rho_{N-1}(\Sigma_N)\,|\,0\rangle, \tag{2.34}$$

where here, and henceforth, we denote σ^x_{Nm} simply by σ^x_m, etc. If we define $K_1{}^*$ as before by

$$\tanh K_1 = e^{-2K_1{}^*} \tag{2.15b}$$

we have

$$\rho_N(\Sigma_N)\,|\,0\rangle = (2\cosh K_1)^M \exp\,(\mathcal{K}_N + \mathcal{K}_N{}^{(2)}) \times \exp\,(-2K_1{}^*\Sigma\sigma^+_m\sigma^-_m)\rho_{N-1}(\Sigma_N)\,|\,0\rangle. \tag{2.35}$$

Let us now consider tr $\rho_N(\Sigma_N)$ in the representation in which all spins are in the $\pm z$ directions. We notice that any product of one or more distinct σ^x's has no diagonal matrix elements in this representation. Thus only the zeroth-order term in the canonical expansion of $\rho_N(\Sigma_N)$ contributes to the trace, and its contribution is the same for all 2^M states; i.e.,

$$\mathrm{tr}\;\rho_N(\Sigma_N) = 2^M\langle 0\,|\,\rho_N(\Sigma_N)\,|\,0\rangle, \tag{2.36}$$

justifying our remark that knowledge of $\rho_N(\Sigma_N)\,|\,0\rangle$ would be sufficient.

Finally we consider possible choices for ρ_0, each one of which defines a slightly different physical problem. The simplest choice, in which the zeroth row is in a thermal reservoir at infinite temperature is (if we normalize ρ_0) the constant

$$\rho_0 = (\tfrac{1}{2})^M. \tag{2.37}$$

In this case

$$Z = \langle 0\,|\,(V_2V_3V_1)^N\,|\,0\rangle \tag{2.38}$$

with

$$V_1 = (2\cosh K_1)^M \exp\,(-2K_1{}^*\Sigma\sigma^+_m\sigma^-_m) = (2\sinh 2K_1)^{M/2} \exp\,[-2K_1{}^*\Sigma(\sigma^+_m\sigma^-_m - \tfrac{1}{2})],$$
$$V_2 = \exp\,(K_2\Sigma\sigma^x_m\sigma^x_{m+1}),$$
$$V_3 = \exp\,(H\Sigma\sigma^x_m). \tag{2.39}$$

Another possible choice is

$$\rho_0 = V_2V_3. \tag{2.40}$$

If we let $N \to N-1$, this choice gives an $N \times M$ lattice with no connections to an external reservoir—the classical Ising problem with free edges—which, therefore, has the partition function

$$Z = \langle 0\,|\,(V_2V_3V_1)^{N-1}(V_2V_3)\,|\,0\rangle = \langle 0\,|\,(V_2V_3V_1)^NV^{-1}{}_1\,|\,0\rangle = (2\cosh K_1)^{-M}\langle 0\,|\,(V_2V_3V_1)^N\,|\,0\rangle. \tag{2.41}$$

In either case the σ's are the operators associated with the spins of the last row, in contrast to the τ matrices of the previous section. To obtain the V's of the last section, we must make the canonical transformation

$$\sigma^x_m \to \sigma^z_m$$
$$\sigma^z_m \to -\sigma^x_m$$

and then identify the σ operators with the corresponding τ matrices.

It is again convenient to deal with a symmetric

operator,[18] so we write (2.38) as

$$Z=\langle 0\mid (V_2V_3)^{-\frac{1}{4}}V^N(V_2V_3)^{\frac{1}{4}}\mid 0\rangle, \tag{2.42}$$

where

$$V=(V_2V_3)^{\frac{1}{4}}V_1(V_2V_3)^{\frac{1}{4}}. \tag{2.43}$$

As $N\to\infty$, only the largest eigenvalue of V survives, and factors like $\langle 0\mid (V_2V_3)^{-\frac{1}{4}}\mid \Psi_{\max}\rangle$ have a negligible effect on the free energy per spin, i.e., the slight differences between (2.42) and (2.19) due to the different boundary conditions at the first and last rows are negligible. For convenience we henceforth work with the cyclic analog to (2.42):

$$Z=\operatorname{tr} V^N. \tag{2.44}$$

It should be remarked that spin correlation functions such as (2.4) can be expressed in the transfer matrix formalism quite simply. For example, by similar methods, one easily obtains for the two-spin correlation function

$$\langle\sigma^x_{n',m'}\sigma^x_{nm}\rangle=\operatorname{tr}(\sigma^x_{m'}V^{n'-n}\sigma^x_mV^{N-(n'-n)})/\operatorname{tr}V^N. \tag{2.45}$$

III. EIGENVALUES AND EIGENVECTORS OF THE TRANSFER MATRIX

A. Introduction of Fermion Operators

The operators V_1, V_2, and V_3 involve linear and quadratic forms of the spin raising and lowering operators, which obey the mixed set of commutation-anticommutation rules

$$\begin{aligned}&[\sigma^{\pm}_m,\sigma^{\pm}_n]=0, \qquad m\neq n\\ &\{\sigma^+_m,\sigma^-_m\}=1, \qquad (\sigma^+_m)^2=(\sigma^-_m)^2=0.\end{aligned} \tag{3.1}$$

The part-boson, part-fermion nature of these rules is a principal source of difficulty, because no simple linear transformation among the σ^+'s and σ^-'s, such as would be required to diagonalize a quadratic form, leaves these rules invariant. It is nevertheless well-known how to change such operators to ones obeying a complete set of anticommutation rules. We introduce annihilation and creation operators by the transformation[19]

$$\begin{aligned}C_m&=[\exp(\pi i\sum_1^{m-1}\sigma^+_j\sigma^-_j)]\sigma^-_m;\\ C_m^\dagger&=[\exp(\pi i\sum_1^{m-1}\sigma^+_j\sigma^-_j)]\sigma^+_m.\end{aligned} \tag{3.2}$$

The C's and $C^\dagger$'s are readily seen to be fermion operators. Then

$$C_m^\dagger C_m=\sigma^+_m\sigma^-_m, \tag{3.3}$$

so that the inverse transformation is simply

$$\begin{aligned}\sigma^-_m&=[\exp(\pi i\sum_1^{m-1}C_j^\dagger C_j)]C_m;\\ \sigma^+_m&=[\exp(\pi i\sum_1^{m-1}C_j^\dagger C_j)]C_m^\dagger.\end{aligned} \tag{3.4}$$

Despite its apparently complicated nonlinear structure, this transformation is useful because quadratic forms involving products of operators on the same site, such as occur in V_1, or of operators on adjacent sites, such as occur in V_2, remain quadratic in the new operators. Thus, because of (3.3), V_1 is just

$$V_1=(2\sinh 2K_1)^{M/2}\exp[-2K_1^*\textstyle\sum(C_m^\dagger C_m-\frac{1}{2})]. \tag{3.5}$$

Also, for $m<M$, one finds

$$\begin{aligned}\sigma^+_m\sigma^-_{m+1}&=C_m^\dagger C_{m+1},\\ \sigma^+_m\sigma^+_{m+1}&=C_m^\dagger C_{m+1}^\dagger,\\ \sigma^-_m\sigma^-_{m+1}&=-C_mC_{m+1},\end{aligned} \tag{3.6}$$

so that if each row is assumed to have free ends,

$$V_2=\exp[K_2\sum_1^{m-1}(C_m^\dagger-C_m)(C_{m+1}^\dagger+C_{m+1})]. \tag{3.7}$$

The operator V_3 is not left in any simple form by the transformation to fermion operators, and it is this feature which has prevented the solution of the Ising problem in a magnetic field. Also, if interactions are between other than nearest neighbors, V_2 involves higher-order terms than quadratic. *For these reasons, we are confined to nearest neighbor interactions and, for the rest of this section, to zero external magnetic field.*

If cyclic boundary conditions are imposed, the bond between the last and first spins introduces complications in V_2, because instead of (3.6) we have

$$\begin{aligned}\sigma^+_M\sigma^-_1&=-(-)^{\mathfrak{N}}C_M^\dagger C_1\neq C_M^\dagger C_1\\ \sigma^+_M\sigma^+_1&=-(-)^{\mathfrak{N}}C_M^\dagger C_1^\dagger\neq C_M^\dagger C_1^\dagger\\ \sigma^-_M\sigma^-_1&=(-)^{\mathfrak{N}}C_MC_1\neq -C_MC_1,\end{aligned} \tag{3.8}$$

so that

$$\begin{aligned}V_2=\exp K_2[&\sum_1^{M-1}(C_m^\dagger-C_m)(C_{m+1}^\dagger+C_{m+1})\\ &-(-)^{\mathfrak{N}}(C_M^\dagger-C_M)(C_1^\dagger+C_1)].\end{aligned} \tag{3.9}$$

Here $\mathfrak{N}$ is again the total number operator,

$$\mathfrak{N}=\sum_1^M\sigma^+_m\sigma^-_m=\sum_1^MC_m^\dagger C_m. \tag{3.10}$$

The difficulties created by this more complicated form for V_2 are not insuperable. To see this we observe

[18] Recall that the operator V, which is identical with Montroll and Newell's P, is only one possible symmetrization of the transfer matrix. Another, $V'=V_1^{\frac{1}{2}}(V_2V_3)V_1^{\frac{1}{2}}$, was used by Yang to derive the spontaneous magnetization. The operator V' is diagonalizable with less algebraic manipulation, but the operator V simplifies expressions for the spontaneous magnetization and the two-spin correlation function. Hence we use the latter. This is discussed further at the end of Sec. IV.

[19] This method was known at least as early as 1928 [See P. Jordan and E. Wigner, Z. Physik 47, 631 (1928)] and has been rediscovered many times since. It has been used to change spin operators into fermions [E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. 16, 407 (1961)], to change electrons into bosons with a "hard core" [E. Lieb and D. Mattis, Phys. Rev. 125, 164 (1962); Appendix], and to change hard core bosons into fermions [T. Schultz, J. Math. Phys. 4, 666 (1963)].

that because all terms in V_1 and V_2 involve bilinear products of fermion operators, the evenness or oddness of $\mathfrak{N}$ is conserved:

$$[(-)^{\mathfrak{N}}, V_1]=[(-)^{\mathfrak{N}}, V_2]=0. \quad (3.11)$$

We can consider separately eigenstates of V in which only even numbers of fermions are present, and other states in which only odd numbers are present. Acting on the even states, V_2 is equivalent to the operator

$$V_2^+= \exp [K_2\sum_1^M(C_m^\dagger-C_m)(C_{m+1}^\dagger+C_{m+1})] \quad (3.11a)$$

with

$$C_{M+1}=-C_1 \quad \text{and} \quad C_{M+1}^\dagger=-C_1^\dagger; \quad (3.12a)$$

acting on the odd states, V_2 is equivalent to the operator

$$V_2^-= \exp [K_2\sum_1^M(C_m^\dagger-C_m)(C_{m+1}^\dagger+C_{m+1})] \quad (3.11b)$$

with

$$C_{M+1}=C_1 \quad \text{and} \quad C_{M+1}^\dagger=C_1^\dagger. \quad (3.12b)$$

Thus we are led to seek the eigenvalues and eigenvectors of the operators

$$V^\pm=(2\sinh 2K_1)^{M/2}\exp[\tfrac{1}{2}K_2\sum_1^M(C_m^\dagger-C_m)$$
$$\times(C_{m+1}^\dagger+C_{m+1})]\exp[-2K_1^*\sum_1^M(C_m^\dagger C_m-\tfrac{1}{2})]$$
$$\times\exp[\tfrac{1}{2}K_2\sum_1^M(C_m^\dagger-C_m)(C_{m+1}^\dagger+C_{m+1})], \quad (3.13)$$

the $\pm$ referring to the anticyclic and cyclic definitions of C_{M+1}, $C_{M+1}^\dagger$, respectively. It is understood that the eigenvectors (and eigenvalues) of V consist of those eigenvectors of V^+ having even numbers of fermions and those eigenvectors of V^- having odd numbers of fermions. *The "odd" eigenvectors of V^+ and the "even" eigenvectors of V^- are irrelevant and must be discarded.*

It should be emphasized that this apparent complication arises solely because of the cyclic boundary conditions; with free ends, there is only one operator V to consider. This implies several advantages for the free-end boundary condition, but the price paid through the loss of translational invariance tends to offset these. In this section, we consider only the case that the rows are cyclic.

Our problem then is to diagonalize the product of three exponentials of quadratic forms in fermion operators. This is somewhat, but not impossibly, more complicated than the diagonalization of a single quadratic form. As one might expect, there exists a general linear transformation to a new set of fermion operators of the type

$$\xi_q=\sum_m g_{qm}C_m+h_{qm}C_m^\dagger, \quad (3.14)$$

in terms of which V appears in the simplest form one could hope to obtain

$$V= \exp(-\Sigma\epsilon_q\xi_q^\dagger\xi_q+\text{constant}). \quad (3.15)$$

The problem is simply to determine the transformation matrices g_{qm} and h_{qm}, the one-fermion "energies" ϵ_q, and the unknown constant. There are several ways to proceed; we follow one that in our view consists of just a few simple and natural steps.

Because of the translational symmetry in the exponents of (3.5) and (3.13), the first step is obviously to go to running wave operators by the linear canonical transformation

$$C_m=M^{-\frac{1}{2}}e^{-i\pi/4}\sum_q e^{iqm}\eta_q. \quad (3.16)$$

The factor $\exp(-i\pi/4)$ is introduced for future convenience to ensure real coefficients in all terms of $V^\pm$ when expressed in terms of the η_q's. The anticyclic condition (3.12a) requires that

$$q\equiv l=\pm\pi/M, \pm 3\pi/M, \cdots, \pm(M-1)\pi/M, \quad (3.17a)$$

while the cyclic condition (3.12b) requires that

$$q\equiv k=0, \pm 2\pi/M, \pm 4\pi/M, \cdots, \pm(M-2)\pi/M, \pi. \quad (3.17b)$$

We have assumed for convenience that M is even.

Direct substitution of (3.16) into (3.13) yields $V^\pm$ in the form

$$V^\pm=(2\sinh 2K_1)^{M/2}\prod_{0\le q\le\pi}V_q, \quad (3.18)$$

where the q's are either all l's or all k's. For $q\neq 0$ or π,

$$V_q=(V_{2q})^{\frac{1}{2}}V_{1q}(V_{2q})^{\frac{1}{2}} \quad (3.19a)$$

with

$$V_{1q}= \exp[-2K_1^*(\eta_q^\dagger\eta_q+\eta_{-q}^\dagger\eta_{-q}-1)], \quad (3.19b)$$

and

$$V_{2q}= \exp\{2K_2[(\cos q)(\eta_q^\dagger\eta_q+\eta_{-q}^\dagger\eta_{-q})$$
$$+(\sin q)(\eta_q\eta_{-q}+\eta_{-q}^\dagger\eta_q^\dagger)]\}. \quad (3.19c)$$

For $q=0$,

$$V_0= \exp[-2(K_1^*-K_2)(\eta_0^\dagger\eta_0-\tfrac{1}{2})], \quad (3.20)$$

and for $q=\pi$,

$$V_\pi= \exp[-2(K_1^*+K_2)(\eta_\pi^\dagger\eta_\pi-\tfrac{1}{2})]. \quad (3.21)$$

Because the operators V_q and $V_{q'}$ involve bilinear products of operators that anticommute, they themselves commute and can be diagonalized simultaneously and independently, an enormous simplification. The operators V_0 and V_π are obviously diagonal in the occupation number representation. For more general values of q, the problem reduces to the diagonalization of V_q between the four vectors Φ_0, Φ_q, Φ_{-q}, Φ_{-qq}. The notation is self-explanatory, and the sign of Φ_{-qq} is determined by $\Phi_{-qq}=\eta_{-q}^\dagger\eta_q^\dagger\Phi_0$.

The second step is to observe that the vectors Φ_q and Φ_{-q} are eigenvectors of V_q, being simultaneously eigenvectors of the operators $\eta_q\eta_{-q}$ and $\eta_{-q}^\dagger\eta_q^\dagger$ with eigenvalue zero, and eigenvectors of the operator $\eta_q^\dagger\eta_q+\eta_{-q}^\dagger\eta_{-q}$ with eigenvalue unity. Thus for $q\neq 0$ or π,

$$V_q\Phi_q = \exp(2K_2\cos q)\Phi_q \tag{3.22}$$

and similarly for Φ_{-q}.

The third step is to diagonalize V between the vectors Φ_{-qq} and Φ_0. It is easy to compute the matrix elements of V_{1q} and V_{2q} between these vectors. V_{1q} is already diagonal:

$$V_{1q}=\begin{pmatrix}\exp(-2K_1^*) & 0\\ 0 & \exp(2K_1^*)\end{pmatrix}. \tag{3.23}$$

To compute the matrix elements of $(V_{2q})^{\frac{1}{2}}$ we introduce the pair annihilation and creation operators

$$b^-{}_q=\eta_q\eta_{-q} \quad\text{and}\quad b^+{}_q=\eta_{-q}^\dagger\eta_q^\dagger \tag{3.24}$$

which, in the space of Φ_{-qq} and Φ_0, obey the simple rules of spin-lowering and raising operators. Then, *in this space*, b^- and b^+ are represented by Pauli spin matrices so that

$$\eta_q^\dagger\eta_q+\eta_{-q}^\dagger\eta_{-q}=2b^+{}_qb^-{}_q\equiv b^z{}_q+1 \tag{3.25a}$$

and

$$\eta_q\eta_{-q}+\eta_{-q}^\dagger\eta_q^\dagger=b^x{}_q, \tag{3.25b}$$

so that

$$\begin{aligned}(V_{2q})^{\frac{1}{2}} &= \exp\{K_2[(b^z{}_q+1)\cos q+b^x{}_q\sin q]\}\\ &= \exp(K_2\cos q)\exp(K_2b^z{}_q')\\ &= \exp(K_2\cos q)(\cosh K_2+b^z{}_q'\sinh K_2)\\ &= \exp(K_2\cos q)\\ &\times\begin{pmatrix}\cosh K_2+\sin K_2\cos q & \sinh K_2\sin q\\ \sinh K_2\sin q & \cosh K_2-\sinh K_2\cos q\end{pmatrix},\end{aligned} \tag{3.26}$$

where $b^z{}_q'=b^z{}_q\cos q+b^x{}_q\sin q$ and has the important property that $(b^z{}_q')^2=1$. Combining (3.23) and (3.26), we obtain the matrix of V_q between the vectors Φ_{-qq} and Φ_0 in the form

$$V_q=\exp(2K_2\cos q)\begin{pmatrix}A_q & C_q\\ C_q & B_q\end{pmatrix}, \tag{3.27}$$

where

$$\begin{aligned}A_q &= \exp(-2K_1^*)(\cosh K_2+\sinh K_2\cos q)^2\\ &\quad+\exp(2K_1^*)(\sinh K_2\sin q)^2\\ B_q &= \exp(-2K_1^*)(\sinh K_2\sin q)^2\\ &\quad+\exp(2K_1^*)(\cosh K_2-\sinh K_2\cos q)^2\\ C_q &= (2\sinh K_2\sin q)\\ &\quad\times(\cosh 2K_1^*\cosh K_2-\sinh 2K_1^*\sinh K_2\cos q).\end{aligned}$$

The two eigenvalues are obtained by elementary algebra:

$$\exp(2K_2\cos q)\{\tfrac{1}{2}(A_q+B_q)\pm[(\tfrac{1}{2}(A_q-B_q))^2+C_q^2]^{\frac{1}{2}}\} = \exp(2K_2\cos q)e^{\pm\epsilon_q}, \tag{3.28}$$

where ϵ_q is the positive root of

$$\cosh\epsilon_q=\cosh 2K_2\cosh 2K_1^*-\sinh 2K_2\sinh 2K_1^*\cos q. \tag{3.29}$$

The eigenvectors belonging, respectively, to the upper and lower signs in (3.28) are also obtained by elementary algebra:

$$\begin{aligned}\Psi_0 &= \cos\phi_q\Phi_0+\sin\phi_q\Phi_{-qq},\\ \Psi_{-qq} &= -\sin\phi_q\Phi_0+\cos\phi_q\Phi_{-qq},\end{aligned} \tag{3.30}$$

where ϕ_q is defined modulo π by

$$\tan\phi_q=C_q/(e^{\epsilon_q}-A_q). \tag{3.31}$$

Simple manipulation gives a more convenient definition

$$\tan 2\phi_q=2C_q/(B_q-A_q), \tag{3.32a}$$

which defines ϕ_q modulo $\pi/2$. The solutions of (3.32) that also solve (3.31) satisfy the additional requirement

$$\operatorname{sgn} 2\phi_q=\operatorname{sgn} q. \tag{3.32b}$$

The paired nature of the quadratic forms in (3.19) and the structure of the four eigenvectors are extremely reminiscent of the pair-Hamiltonian and the energy states introduced by Bardeen, Cooper, and Schrieffer[20] in the theory of superconductivity, particularly in Anderson's formulation[21] in which electron-pair operators were in fact formally replaced by spin operators [analogous to our $b^\pm{}_q$ of Eq. (3.24)], in the subspace where pairs were not "broken up." We can simplify the results for V_q in precisely the same way that Bogolubov[11] and Valatin[12] simplified the BCS theory, if we introduce the transformation

$$\begin{aligned}\xi_q &= \cos\phi_q\eta_q+\sin\phi_q\eta_{-q}^\dagger,\\ \xi_{-q} &= \cos\phi_q\eta_{-q}-\sin\phi_q\eta_q^\dagger.\end{aligned} \tag{3.33}$$

Then it is readily verified that the four eigenvectors are defined by

$$\begin{aligned}&\xi_q\Psi_0=\xi_{-q}\Psi_0=0, \qquad \Phi_q\equiv\Psi_q=\xi_q^\dagger\Psi_0,\\ &\Phi_{-q}\equiv\Psi_{-q}=\xi_{-q}^\dagger\Psi_0, \qquad \Phi_{-qq}=\xi_{-q}^\dagger\xi_q^\dagger\Psi_0.\end{aligned} \tag{3.34}$$

In terms of the ξ-operators, V_q becomes

$$V_q=\exp(2K_2\cos q)\exp[-\epsilon_q(\xi_q^\dagger\xi_q+\xi_{-q}^\dagger\xi_{-q}-1)]. \tag{3.35}$$

[20] J. Bardeen, L. Cooper, and J. Schrieffer, Phys. Rev. 108, 1175 (1957).

[21] P. W. Anderson, Phys. Rev. 112, 1900 (1958).

The special cases $q=0$ and $q=\pi$ can also be written in this notation if we define

$$\phi_0=0 \quad \text{and} \quad \epsilon_0=2(K_1^*-K_2) \tag{3.36a}$$

$$\phi_\pi=0 \quad \text{and} \quad \epsilon_\pi=2(K_1^*+K_2), \tag{3.36b}$$

so that

$$V_0V_\pi=\exp\left[2K_2(\cos 0+\cos\pi)\right] \times\exp\left[-\epsilon_0(\xi_0^\dagger\xi_0-\tfrac{1}{2})-\epsilon_\pi(\xi_\pi^\dagger\xi_\pi-\tfrac{1}{2})\right]. \tag{3.37}$$

We thus obtain the extremely simple form for $V^\pm$:

$$V^\pm=(2\sinh 2K_1)^{M/2}\exp\left[-\sum_{\text{all } q}\epsilon_q(\xi_q^\dagger\xi_q-\tfrac{1}{2})\right], \tag{3.38}$$

where we have used the fact that $2K_2\sum\cos q=0$.

It is to be noted that a state with an even (odd) number of ξ-particles involves only even (odd) numbers of η-particles. *Thus the allowable eigenstates of V^+ must have even numbers of ξ-particles; of V^-, odd numbers of ξ-particles.* We denote the eigenstates of V^+ and V^- by Ψ^+ and Ψ^- whenever it is useful to distinguish them.

It is also important to observe that for $T\neq T_c$,

$$\epsilon_q\geq\epsilon_{\min}>0, \qquad q\neq 0$$

and

$$\epsilon_0=\pm\lim_{q\to 0}\epsilon_q\gtrless 0 \quad \text{for} \quad T\gtrless T_c. \tag{3.39}$$

Here T_c is defined by $K_1^*=K_2$, or equivalently, by Eq. (2.15b),

$$\sinh(2J_1/kT_c)\sinh(2J_2/kT_c)=1, \tag{3.40}$$

the famous relation for the transition temperature, first derived for the square lattice by Kramers and Wannier[13] prior to Onsager's exact solution.

The partition function, from which one immediately obtains all the well-known thermodynamic properties of the two-dimensional Ising model, is just the Nth power of the largest eigenvalue of V, in analogy with the one-dimensional case.[22] The fact that the other eigenvalues have negligible effect when N, $M\to\infty$ is shown in the argument leading to Eq. (5.21) of Sec. VB. Let us then inquire into the maximum eigenvalue and the corresponding "maximum eigenvector."

The maximum eigenvalue of V^+ is for the ξ_l-particle vacuum, Ψ^+_0, and is

$$\Lambda^+_0=(2\sinh 2K_1)^{M/2}\exp\left[\tfrac{1}{2}\sum_l\epsilon_l\right]. \tag{3.41}$$

The eigenvector Ψ^+_0, having an even number of ξ_l-particles, is allowable and is therefore an eigenvector of V. All other eigenvalues of V^+ are less than Λ^+_0 by factors like $\exp(-\epsilon_{\min})$ or smaller.

The maximum eigenvalue of V^- is either for the ξ_k-particle vacuum, Ψ^-_0, or for the eigenvector with the $k=0$ particle present, $\Psi^-_{k=0}=\xi_{k=0}^\dagger\Psi^-_0$, depending on whether $\epsilon_{k=0}$ is, respectively, positive or negative (i.e., whether $T>T_c$ or $T<T_c$). The largest eigenvalue of V^- in both cases is

$$\Lambda^-_0 \text{ (or, respectively, } \Lambda^-_{k=0})=(2\sinh 2K_1)^{M/2} \times\exp\left[\tfrac{1}{2}\sum_k|\epsilon_k|\right], \tag{3.42}$$

and again all other eigenvalues of V^- are less by factors of $\exp(-\epsilon_{\min})$ or smaller.

Above T_c the maximum eigenvector Ψ^-_0, containing an even number of ξ_k-particles, is not allowable, so the maximum eigenvalue of V is just Λ^+_0 and is non-degenerate. Below T_c, the maximum eigenvector $\Psi^-_{k=0}$, containing an odd number of ξ_k-particles, is also allowable. The two maximum eigenvalues of V, Λ^+_0 and $\Lambda^-_{k=0}$ contain sums that are both approximations to

$$\frac{M}{2\pi}\int_{-\pi}^{\pi}\epsilon_q dq,$$

the integral of a periodic analytic function. The errors in the approximations are both exponentially small[23] for large M, as Onsager originally remarked, because all correction terms in the Euler–MacLaurin expansion vanish. Thus the largest eigenvalues of V^+ and V^- are exponentially degenerate in the limit $M\to\infty$. We call them simply Λ_0:

$$\Lambda_0=(2\sinh 2K_1)^{M/2}\exp\left(\frac{M}{4\pi}\int_{-\pi}^{\pi}\epsilon_q dq\right). \tag{3.43}$$

The effect on the free energy per spin of this degeneracy is $N^{-1}\ln 2$, i.e., negligible, so that one obtains

$$F=-kT\left[\ln(2\sinh 2K_1)^{\frac{1}{2}}+\frac{1}{4\pi}\int_{-\pi}^{\pi}\epsilon_q\,dq\right]. \tag{3.44}$$

The degeneracy nevertheless plays an important role in the long-range order, as was first shown by Ashkin and Lamb,[24] and as we see in Sec. V.

We need not repeat how (3.44) can be written in a form that brings out the similarity between K_1 and K_2, how it leads to a logarithmic singularity in the specific heat, etc., subjects which are discussed by Onsager, Domb, Newell and Montroll, and Huang.[25]

IV. SPIN-SPIN CORRELATION FUNCTION

We consider now the evaluation of the correlation function between two spins in the same row:

$$\langle\sigma^x_{nm}\sigma^x_{nm'}\rangle= \lim_{M,N\to\infty}\operatorname{tr}\sigma^x_{nm}\sigma^x_{nm'}\exp(-\beta\mathcal{H}_0)/\operatorname{tr}\exp(-\beta\mathcal{H}_0). \tag{4.1}$$

Expressed in the transfer matrix formalism, this is

$$\langle\sigma^x_{nm}\sigma^x_{nm'}\rangle=\lim_{M,N\to\infty}(\operatorname{tr}\sigma^x_m\sigma^x_{m'}\cdot V^N/\operatorname{tr}V^N). \tag{4.2}$$

[22] If the largest eigenvalue is twofold degenerate, as it is for $T<T_c$, the partition function is increased by a factor of two, making a negligible change in the free-energy per spin.

[23] See remark of Domb, Ref. 2, p. 194.

[24] J. Ashkin and W. E. Lamb, Phys. Rev. 64, 159 (1943).

[25] K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, London, 1963), pp. 369 ff.

If we expand in the eigenvectors of V belonging to the eigenvalues Λ_α, we have

$$\langle \sigma^x_m \sigma^x_{m'} \rangle = \lim_{M,N\to\infty} [(\sum_\alpha \langle \Psi_\alpha \mid \sigma^x_m \sigma^x_{m'} \mid \Psi_\alpha \rangle \Lambda_\alpha{}^N)/\sum_\alpha \Lambda_\alpha{}^N]. \quad (4.3)$$

It is shown in Sec. VB that only the eigenvector(s) belonging to the largest eigenvalue of V contribute in the numerator and denominator when we take the limit M, $N\to\infty$. Thus, for $T<T_c$, when $M\to\infty$,

$$\langle \sigma^x_m \sigma^x_{m'} \rangle = \lim_{M\to\infty} \tfrac{1}{2}[\langle \Psi^+_0 \mid \sigma^x_m \sigma^x_{m'} \mid \Psi^+_0 \rangle_M + \langle \Psi^-_{k=0} \mid \sigma^x_m \sigma^x_{m'} \mid \Psi^-_{k=0} \rangle_M]. \quad (4.4)$$

The two expectation values depend on M through the eigenvectors. We now consider the first of these in detail, and then show that the two are equal.

The evaluation is made easy if we write the product $\sigma^x_m \sigma^x_{m'}$ in terms of fermion operators. From the original transformation (3.4) we have

$$\sigma^x_m \sigma^x_{m'} = C^x_m [\exp(\pi i \sum_m^{m'-1} C_j{}^\dagger C_j)] C^x_{m'} = (iC^y_m)[\exp(\pi i \sum_{m+1}^{m'-1} C_j{}^\dagger C_j)] C^x_{m'}, \quad (4.5a)$$

where

$$C^x_j = C_j{}^\dagger + C_j \quad \text{and} \quad iC^y_j = C_j{}^\dagger - C_j. \quad (4.5b)$$

Observing that

$$(-)^{C_j{}^\dagger C_j} = (C_j{}^\dagger + C_j)(C_j{}^\dagger - C_j) = C^x_j (iC^y_j), \quad (4.6)$$

we obtain the product of $2(m'-m)$ fermion operators

$$\sigma^x_m \sigma^x_{m'} = (iC^y_m)(C^x_{m+1})(iC^y_{m+1}) \cdots (C^x_{m'-1}) \times (iC^y_{m'-1})(C^x_{m'}). \quad (4.7)$$

To evaluate the "vacuum" expectation value of this product, we use Wick's theorem, which states that we must associate the operators in pairs (with the operators of each pair written in the original order), replace each pair by its contraction (in this case, vacuum expectation value), multiply the product of these contractions by $(-)^p$ [where $(-)^p$ is the signature of the permutation necessary to bring paired operators next to each other from the original ordering], and sum these products over all pairings. The three kinds of contractions that occur are readily evaluated if we combine the transformation (3.16) and the inverse of (3.33):

$$C_m = M^{-\frac{1}{2}} e^{-i\pi/4} \sum_q e^{iqm}(\cos\phi_q \xi_q - \sin\phi_q \xi_{-q}{}^\dagger) \quad (4.8)$$

with

$$\phi_{-q} \equiv -\phi_q. \quad (4.9)$$

The q's range over either the set of l's or the set of k's, whichever is more convenient. Then[26]

$$\langle \Psi^+_0 \mid C^x_i C^x_j \mid \Psi^+_0 \rangle = \langle \Psi^+_0 \mid C^y_i C^y_j \mid \Psi^+_0 \rangle = 0, \quad i\neq j \quad (4.10)$$

and

$$\langle \Psi^+_0 \mid iC^y_i C^x_j \mid \Psi^+_0 \rangle = -M^{-1} \sum_l \exp[il(i-j)] \exp(-i2\phi_l). \quad (4.11)$$

If one defines

$$a_{ij} = \langle \Psi^+_0 \mid iC^y_i C^x_{j+1} \mid \Psi^+_0 \rangle, \quad (4.12)$$

then the sum over all pairings is

$$\langle \Psi^+_0 \mid \sigma^x_m \sigma^x_{m'} \mid \Psi^+_0 \rangle = \sum_P (-)^P a_{m,Pm} \cdots a_{m'-1,P(m'-1)} = \begin{vmatrix} a_{m,m} & a_{m,m+1} & \cdots & a_{m,m'-1} \\ a_{m+1,m} & & & \vdots \\ \vdots & & & \\ a_{m'-1,m} & & \cdots & a_{m'-1,m'-1} \end{vmatrix}, \quad (4.13)$$

i.e., the correlation function between two spins $m'-m$ sites apart in the same row is a determinant of order $m'-m$. For the cyclic problem we are considering, we see that

$$a_{ij} = a_{j-i} = -M^{-1} \sum_l \exp[-il(j-i)] \exp[-i(2\phi_l + l)], \quad (4.14)$$

so that the determinant in (4.13) is a Toeplitz determinant (the ijth element depends only on $i-j$) and its asymptotic behavior can be calculated by a theorem of Szegö[27] as generalized and applied by Montroll, Potts, and Ward (MPW).[10] In fact, the determinant (4.13) with the definition (4.14) is identical with theirs, so we do not need to repeat its evaluation.

To see the identity of a_{j-i} defined by (4.14) and MPW's a_r, we need an explicit expression for $\exp(-i2\phi_q)$. From (3.32a) one obtains

$$\exp(-i4\phi_l) = \frac{e^{2il} - 2\,\mathrm{ctnh}\,2K_1{}^*\,\mathrm{ctnh}\,K_2 e^{il} + \mathrm{ctnh}^2 K_2}{e^{-2il} - 2\,\mathrm{ctnh}\,2K_1{}^*\,\mathrm{ctnh}\,K_2 e^{-il} + \mathrm{ctnh}^2 K_2},$$

[26] This situation is identical to what we found for the "XY model" of quantum mechanical spins in one dimension, where it is discussed in more detail. See E. Lieb, D. Mattis, and T. Schultz, Ann. Phys. 16, 407 (1961), especially pp. 417 ff.

[27] See V. Grenander and G. Szegö, *Toeplitz Forms and their Applications* (University of California Press, Berkeley, California, 1958). For a proof that is extendable to non-Hermitian kernels, as is the case here, see M. Kac, *Probability and Related Topics in Physical Sciences* (Interscience Publishers, Inc., New York, 1959).

which can be written in factored form as

$$\exp(-i4\phi_l)=\frac{(e^{il}-x_1)(e^{il}-x_2)}{(e^{-il}-x_1)(e^{-il}-x_2)}, \quad (4.15)$$

with

$$x_1=\operatorname{ctnh} K_1^* \operatorname{ctnh} K_2>1$$

and

$$x_2=(\operatorname{ctnh} K_2/\operatorname{ctnh} K^*_1)\gtrless 1 \quad \text{for} \quad T\gtrless T_c. \quad (4.16)$$

The appropriate square root of (4.15) consistent with the requirement (3.32b) is

$$\exp(-i2\phi_l)$$

$$=e^{il}\left[\frac{(1-x_1^{-1}e^{il})(1-x_2e^{-il})}{(1-x_1^{-1}e^{-il})(1-x_2e^{il})}\right]^{\frac{1}{2}} \quad \text{for} \quad T<T_c, \quad (4.17a)$$

$$=-\left[\frac{(1-x_1^{-1}e^{il})(1-x_2^{-1}e^{il})}{(1-x_1^{-1}e^{-il})(1-x_2^{-1}e^{-il})}\right]^{\frac{1}{2}} \quad \text{for} \quad T>T_c, \quad (4.17b)$$

where the phase angles of all four factors on the right are taken to be in $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$.

If we identify

$$2\phi_l+l=\delta^*(l), \quad (4.18)$$

then in the limit $M\to\infty$, the elements a_{j-i} and the determinant (4.18) agree exactly with those obtained by Montroll, Potts, and Ward.[28]

The analysis of $\langle\Psi^-_{k=0}\,|\,\sigma^x_m\sigma^x_{m'}\,|\,\Psi^-_{k=0}\rangle$ proceeds in exactly the same way, with all contractions being defined as expectation values in the state $\Psi^-_{k=0}$, rather than in Ψ^+_0. The $k=0$ term in the sum corresponding to (4.14) changes sign, but in the limit $M\to\infty$, this has no effect on a_{j-i}. Therefore

$$\langle\Psi^-_{k=0}\,|\,\sigma^x_m\sigma^x_{m'}\,|\,\Psi^-_{k=0}\rangle=\langle\Psi^+_0\,|\,\sigma^x_m\sigma^x_{m'}\,|\,\Psi^+_0\rangle, \quad (4.19)$$

as asserted earlier.

Below the critical temperature, the asymptotic value of the determinant (4.13) is evaluated by MPW using Szegö's theorem. It turns out to be

$$\lim_{m'-m\to\infty}\lim_{M,N\to\infty}\langle\sigma^x_{nm}\sigma^x_{nm'}\rangle_{MN}$$

$$=\left[1-\frac{(1-\tanh^2 K_1)^2(1-\tanh^2 K_2)^2}{16\tanh^2 K_1\tanh^2 K_2}\right]^{\frac{1}{4}}. \quad (4.20)$$

A remarkable property of this correlation function is that it is symmetric in J_1 and J_2; *the two-spin correlation function along a row and along a column are asymptotically equal even in an anisotropic lattice.*

Above the critical temperature, the asymptotic value can be shown to be zero directly by similar methods,[29] or indirectly by using the results proved in Sec. VA.

It is interesting to recall that Kaufman and Onsager, using similar algebraic methods, nevertheless derived the two-spin correlation function as the sum of two determinants rather than as a single determinant, and that Montroll, Potts, and Ward proved the equivalence of the two results only with considerable effort. The reason for the two possible forms, and their identity, can be seen immediately within the algebraic formalism. The Kaufman and Onsager result, rather than the single determinant, is obtained if one works with the transfer matrix V',

$$V'=V_1^{\frac{1}{2}}V_2V_1^{\frac{1}{2}}, \quad (4.21)$$

which differs from V only in the way it is symmetrized. Then a similar diagonalization procedure can be followed, leading to a canonical transformation analogous to (4.8) but with an angle ϕ_q' rather than ϕ_q, defined by

$$\tan 2\phi_q'=\frac{\sinh 2K_2\sin q}{\sinh 2K_1^*\cosh 2K_2-\cosh 2K_1^*\sinh 2K_2\cos q}, \quad (4.22a)$$

with the requirement

$$\operatorname{sgn} 2\phi_q'=\operatorname{sgn} q. \quad (4.22b)$$

Instead of (4.2) the correlation function takes the form

$$\langle\sigma^x_{nm}\sigma^x_{nm'}\rangle=\lim_{M,N\to\infty}\frac{\operatorname{tr} V_1^{-\frac{1}{2}}\sigma^x_m\sigma^x_{m'}V_1^{\frac{1}{2}}V'^N}{\operatorname{tr} V'^N}, \quad (4.23)$$

so that one must consider the expectation value

$$\langle\Psi^+_0{}'\,|\,(V_1^{-\frac{1}{2}}\sigma^x_mV_1^{\frac{1}{2}})(V_1^{-\frac{1}{2}}\sigma^x_{m'}V_1^{\frac{1}{2}})\,|\,\Psi^+_0{}'\rangle_M$$

$$=\langle\Psi^+_0{}'\,|\,(\sigma^x_m\cosh K_1^*+i\sigma^y_m\sinh K_1^*)$$

$$\times(\sigma^x_{m'}\cosh K_1^*+i\sigma^y_{m'}\sinh K_1^*)\,|\,\Psi^+_0{}'\rangle_M, \quad (4.24)$$

and a corresponding one for $\Psi^-_{k=0}{}'$, which can be shown to be the same when $M\to\infty$. $\Psi^+_0{}'$ is obviously the eigenvector of V' corresponding to Ψ^+_0 for V, etc.

Of the four terms of the product in (4.24), only the terms involving $\sigma^x_m\sigma^x_{m'}$ and $\sigma^y_m\sigma^y_{m'}$ have nonzero expectation values [the other two terms, when simplified using Wick's theorem, always involve a factor of the form $\langle\Psi^+_0{}'\,|\,C^x_iC^x_j\,|\,\Psi^+_0{}'\rangle$ or $\langle\Psi^+_0{}'\,|\,C^y_iC^y_j\,|\,\Psi^+_0{}'\rangle$, $i\neq j$, which vanish as in Eq. (4.10)], so we obtain

$$\langle\sigma^x_{nm}\sigma^x_{nm'}\rangle=\cosh^2 K_1^*\langle\Psi^+_0{}'\,|\,\sigma^x_m\sigma^x_{m'}\,|\,\Psi^+_0{}'\rangle_{M\to\infty}$$

$$+\sinh^2 K_1^*\langle\Psi^+_0{}'\,|\,(i\sigma^y_m)(i\sigma^y_{m'})\,|\,\Psi^+_0{}'\rangle_{M\to\infty}. \quad (4.25)$$

The two expectation values on the right lead to the two determinants of Kaufman and Onsager.

[28] In $\delta^*(l)$ for $T<T_c$, a term equal to π has been omitted by MPW, but this does not affect the conclusion. Also, to make the agreement manifest, we must interchange K_1 and K_2, K_1^* and K_2^*, etc.

[29] Dr. Montroll and Dr. Potts have kindly informed us that their use of the Szegö-Kac theorem in this case is not correct as it appears in MPW, but that it can be corrected.

With T.D. Schultz and D.C. Mattis in Rev. Mod. Phys. *36*, 856–871 (1964)

V. SPONTANEOUS MAGNETIZATION

A. General Remarks

In contrast to the free energy, the spontaneous magnetization of the Ising model on a square lattice, correctly defined, has never been solved with complete mathematical rigor. Starting from the only sensible definition of the spontaneous magnetization, the methods of Yang, and of Montroll, Potts, and Ward are each forced to make an assumption that has not been rigorously justified. The assumptions appear to be quite different; however, from the similarities between the difficulties encountered in trying to justify them, and the identity of the results obtained, one might conclude that they are closely related. In this section we discuss these assumptions; in the following two sections we discuss the MPW and Yang approaches, respectively, in more detail.

Ordinarily in statistical mechanics, the kind of mathematical questions we wish to examine *are completely ignored.* But in the Ising model, which is exactly soluble in certain respects, it is rewarding to be more careful, and to see precisely what one must assume even here.

For a finite lattice in a magnetic field $\mathfrak{H}$ (in the x direction), the free energy per site and the magnetization (magnetic moment per site) are defined by

$$F_{MN}(\mathfrak{H}) = -(1/\beta MN) \ln \operatorname{tr} \exp(-\beta \mathcal{H}_0) \exp(\beta \mathfrak{H} \sum \sigma^x_{mn}) \quad (5.1)$$

and

$$\mathfrak{M}_{MN}(\mathfrak{H}) = \frac{1}{MN} \frac{\operatorname{tr} \sum \sigma^x_{mn} \exp(-\beta \mathcal{H}_0) \exp(\beta \mathfrak{H} \Sigma \sigma^x_{ij})}{\operatorname{tr} \exp(-\beta \mathcal{H}_0) \exp(\beta \mathfrak{H} \Sigma \sigma^x_{ij})} = -\partial F_{MN}/\partial \mathfrak{H}, \quad (5.2)$$

where $\mathcal{H}_0$ is the Hamiltonian in the absence of a field, and again we have set the Bohr magneton equal to unity. The spontaneous magnetization is in some sense the limit of the magnetization when $\mathfrak{H} \to 0+$, but considerable care must be taken with the limit. Thus, it is clear that the spontaneous magnetization is *not* obtained from

$$\lim_{\mathfrak{H} \to 0+} \mathfrak{M}_{MN}(\mathfrak{H}),$$

which vanishes for all finite M and N, as can be seen by expanding each term of (5.2) in powers of $\mathfrak{H}$. For finite M and N, $F_{MN}(\mathfrak{H})$ is analytic for all real $\mathfrak{H}$ and is quadratic in $\mathfrak{H}$ for sufficiently small $\mathfrak{H}$.

The correct definition of the spontaneous magnetization requires that $\lim_{M,N\to\infty}$ be taken *before* $\lim_{\mathfrak{H}\to 0+}$. That is, *the spontaneous magnetization is defined by*

$$\mathfrak{M}_s = \lim_{\mathfrak{H}\to 0+} \lim_{M,N\to\infty} \mathfrak{M}_{MN}(\mathfrak{H}), \quad (5.3)$$

which definition we take as fundamental. Physically, this definition corresponds to the experimental situation, in which $\mathfrak{H}$ is allowed to become small on a macroscopic scale and $\mathfrak{M}_s$ is the extrapolation of the $\mathfrak{M}(\mathfrak{H})$ curve. The values of $\mathfrak{H}$ determining the extrapolated value are all much greater than M^{-1} or N^{-1} (in units of kT/μ_{Bohr}), so that one must pass to the limit $M, N \to \infty$ *before* letting $\mathfrak{H}$ tend to zero. Mathematically, although the sequence of functions $F_{MN}(\mathfrak{H})$ are all quadratic in $\mathfrak{H}$, for small $\mathfrak{H}$, the limit function

$$F(\mathfrak{H}) = \lim_{M,N\to\infty} F_{MN}(\mathfrak{H}) \quad (5.4)$$

may vary as $|\mathfrak{H}|$ for small $\mathfrak{H}$, and just such a behavior would lead to spontaneous magnetization. Unfortunately, no one has succeeded in calculating the function $F(\mathfrak{H})$ for $\mathfrak{H} \neq 0$.

As we shall see in Sec. VC, Yang calculated a quantity $\mathfrak{M}_{\text{Yang}}$ defined by a different limiting process:

$$\mathfrak{M}_{\text{Yang}} = |\lim_{\alpha\to 0+} \lim_{\substack{M,N\to\infty \\ \mathfrak{H}=\alpha/M}} \mathfrak{M}_{MN}(\mathfrak{H})|. \quad (5.5)$$

It has not been possible to show the equivalence of Eq. (5.5) with the spontaneous magnetization as given by the fundamental definition. We have, however, been able to show that if one takes the limit $\alpha \to \infty$ instead of $\alpha \to 0$, in Eq. (5.5), then the resulting expression is the spontaneous magnetization. Unfortunately, the expression $\lim_{M,N\to\infty} \mathfrak{M}_{MN}(\alpha/M)$ has only been computed for α very small.

The important reason why Yang's definition appears to agree with the fundamental one is that the quadratic dependence of $F_{MN}(\mathfrak{H})$ persists as $\mathfrak{H}$ increases only so long as $\mathfrak{H} = O(1/MN)$; for larger $\mathfrak{H}$, $F_{MN}(\mathfrak{H})$ appears to be linear in $\mathfrak{H}$, and presumably the slope is the same for $\mathfrak{H} = O(1/M)$ and for $\mathfrak{H} = O(1)$.

In order to verify this quadratic behavior for $\mathfrak{H} = O(1/MN)$ and to obtain a third possible definition for spontaneous magnetization on which both the calculations of Yang and of MPW can be based, it is useful to consider the probability density that the magnetization have the value $\mathfrak{M}$ in the absence of a magnetic field:

$$p_{MN}(\mathfrak{M})\, d\mathfrak{M} = \sum_{S(\mathfrak{M})} \exp(-\beta \mathcal{H}_0) / \sum_{\text{all states}} \exp(-\beta \mathcal{H}_0), \quad (5.6)$$

where $S(\mathfrak{M})$ is the set of all states for which

$$\mathfrak{M} < (MN)^{-1} \sum_{nm} \sigma^x_{nm} < \mathfrak{M} + d\mathfrak{M}.$$

The limiting density is defined as

$$p(\mathfrak{M}) = \lim_{M,N\to\infty} p_{MN}(\mathfrak{M}). \quad (5.7)$$

$p_{MN}(\mathfrak{M})$ is even in $\mathfrak{M}$ by symmetry. Also, because it is the probability density of a macroscopic quantity, one expects it to peak sharply at points we shall call $\pm\mathfrak{M}_0$ and which we subsequently identify with $\pm\mathfrak{M}_s$.[30]

[30] Above the critical temperature, of course, there is only one sharp peak around $\mathfrak{M}_0 = 0$.

The magnetization in a field $\mathfrak{H}$ is then

$$\mathfrak{M}_{MN}(\mathfrak{H})=\frac{\int_{-\infty}^{\infty}\mathfrak{M}p_{MN}(\mathfrak{M})\exp(\beta\mathfrak{H}\mathfrak{M}MN)\,d\mathfrak{M}}{\int_{-\infty}^{\infty}p_{MN}(\mathfrak{M})\exp(\beta\mathfrak{H}\mathfrak{M}MN)\,d\mathfrak{M}}$$

$$=\frac{\int_{0}^{\infty}\mathfrak{M}p_{MN}(\mathfrak{M})\sinh(\beta\mathfrak{H}\mathfrak{M}MN)\,d\mathfrak{M}}{\int_{0}^{\infty}p_{MN}(\mathfrak{M})\cosh(\beta\mathfrak{H}\mathfrak{M}MN)\,d\mathfrak{M}}. \quad (5.8)$$

The quadratic behavior for extremely small $\mathfrak{H}$ follows if $p_{MN}(\mathfrak{M})$ satisfies the very weak condition that it be negligible for $\mathfrak{M}>\mathfrak{M}_0\times$(constant of order unity). Then, if $0<\mathfrak{H}\ll(\beta\mathfrak{M}_0MN)^{-1}=O(1/MN)$, we can expand the hyperbolic functions in (5.8) obtaining

$$\mathfrak{M}(\mathfrak{H})=(\beta\mathfrak{H}MN)\int_0^\infty\mathfrak{M}^2p(\mathfrak{M})\,d\mathfrak{M}\Big/\int_0^\infty\mathfrak{M}p(\mathfrak{M})\,d\mathfrak{M}$$

$$=\beta\mathfrak{H}MN\langle\mathfrak{M}^2\rangle/\langle|\mathfrak{M}|\rangle; \quad (5.9)$$

corresponding to the quadratic dependence of $F_{MN}(\mathfrak{H})$ on $\mathfrak{H}$. We note that in this linear region of the magnetization curve, the susceptibility is proportional to the size of the lattice.

For $\mathfrak{H}$ of macroscopic size, the hyperbolic functions in (5.8) differ negligibly from $2\exp(\beta\mathfrak{H}\mathfrak{M}MN)$ so that we can write

$$\mathfrak{M}_{MN}(\mathfrak{H})$$

$$=\frac{\int_0^\infty\mathfrak{M}p_{MN}(\mathfrak{M})\exp[\beta\mathfrak{H}(\mathfrak{M}-\mathfrak{M}_0)MN]\,d\mathfrak{M}}{\int_0^\infty p_{MN}(\mathfrak{M})\exp[\beta\mathfrak{H}(\mathfrak{M}-\mathfrak{M}_0)MN]\,d\mathfrak{M}}. \quad (5.10)$$

Now, only for an *extremely* sharply peaked $p_{MN}(\mathfrak{M})$, an example of which might be the form

$$p_{MN}(\mathfrak{M})\sim\exp[-A(\mathfrak{M}-\mathfrak{M}_0)^2]$$

$$+\exp[-A(\mathfrak{M}+\mathfrak{M}_0)^2],\quad\text{with } A=O(MN), \quad (5.11)$$

will the effect of the exponentials in Eq. (5.10) for small but macroscopic $\mathfrak{H}$ be small.[31] Then, we would obtain

$$\mathfrak{M}_s=\lim_{\mathfrak{H}\to0+}\lim_{M,N\to\infty}\mathfrak{M}_{MN}(\mathfrak{H})=\langle|\mathfrak{M}|\rangle$$

$$=\lim_{M,N\to\infty}2\int_0^\infty\mathfrak{M}p_{MN}(\mathfrak{M})\,d\mathfrak{M}. \quad (5.12)$$

[31] It should be remarked that an ansatz like (5.11) is *much* stronger than the more usual requirement $\langle(\mathfrak{M}-\langle\mathfrak{M}\rangle)^2\rangle=O(1/MN)$ or even analogous requirements on any higher moments up to moments of order MN.

If $p_{MN}(\mathfrak{M})$ is so strongly peaked, it is more convenient to calculate $\mathfrak{M}$, from

$$\mathfrak{M}_s^2=\langle\mathfrak{M}^2\rangle=\lim_{M,N\to\infty}2\int_0^\infty\mathfrak{M}^2p_{MN}(\mathfrak{M})\,d\mathfrak{M}, \quad (5.13)$$

which can be considered as a third definition of the spontaneous magnetization. Although the MPW calculation has been, and the Yang calculation can be, based on this definition, it has not been possible to show rigorously that it is equivalent to (5.3), i.e., that $p_{MN}(\mathfrak{M})$ *is* sufficiently peaked.

Let us turn to a more detailed consideration of (5.13), deriving both the MPW method and the Yang method.

B. Spontaneous Magnetization and Long-Range Order

Definition (5.13) for $\mathfrak{M}_s$, when written explicitly, is

$$\mathfrak{M}_s^2=\lim_{M,N\to\infty}\langle[(MN)^{-1}\textstyle\sum\sigma^x_{nm}]^2\rangle_{MN}$$

$$=\lim_{M,N\to\infty}(MN)^{-2}\sum_{nmn'm'}\langle\sigma^x_{n'm'}\sigma^x_{nm}\rangle_{MN}, \quad (5.14)$$

where $\langle\cdots\rangle_{MN}$ denotes a thermal average in zero field for an $M\times N$ lattice. For the cyclic problem, the thermal average of (5.14) depends only on $n'-n$ and $m'-m$, so we can write

$$\mathfrak{M}_s^2=\lim_{M,N\to\infty}(MN)^{-1}\sum_{m'n'}\langle\sigma^x_{n'm'}\sigma^x_{nm}\rangle_{MN}. \quad (5.15)$$

This is the starting point of Montroll, Potts, and Ward. Their use of (5.15) has rested on the observation that the terms in the sum $\sum_{m'n'}$ for $m'-m$ and $n'-n$ less than some large value do not survive the multiplication by $(MN)^{-1}$ and the limit $M, N\to\infty$. One has therefore to consider the long-range order $\langle\sigma^x_{n'm'}\sigma^x_{nm}\rangle_{MN}$ for $M, N\to\infty$ and $n'-n$, $m'-m$ large.

Actually, there are at least two kinds of long-range order: the "*short* long-range order" defined by

$$f(\alpha)=\lim_{\substack{r,s\to\infty\\ s/r=\tan\alpha}}\lim_{M,N\to\infty}\langle\sigma^x_{n+s,m+r}\sigma^x_{nm}\rangle_{MN} \quad (5.16)$$

and calculated for $\alpha=0$ in the previous section, and the "*long* long-range order" defined by

$$g(\mu,\nu)=\lim_{M,N\to\infty}\langle\sigma^x_{n+\nu N,m+\mu M}\sigma^x_{nm}\rangle_{MN},\qquad 0<\mu,\nu<1. \quad (5.17)$$

Previously it has first been assumed that (5.15) can be written in terms of the short long-range order, when in fact it is the long long-range order that ultimately enters in (5.15). It has second been found necessary to assume that $f(\alpha)$ is independent of α, because only for $\alpha=0$ (or $\alpha=\frac{1}{2}\pi$) has $f(\alpha)$ been easy to calculate. The first assumption has been made without any justification. The second is suggested (but hardly proved) by the fact that the explicit calculation (as we have observed) gives $f(0)=f(\frac{1}{2}\pi)$, even for the ani-

sotropic case $J_1 \neq J_2$. We now prove these two assumptions by showing that

$$g(\mu,\nu)\equiv g, \qquad \text{all } \mu>0,\ \nu>0, \tag{5.18a}$$

and

$$f(\alpha)\equiv g, \qquad \text{all } \alpha. \tag{5.18b}$$

Thus[32]

$$\mathfrak{M}_s^2=\int_0^1\int_0^1 d\mu\, d\nu\, g(\mu,\nu)=f(0), \tag{5.19}$$

the basic formula usually assumed.

For fixed M and N, we consider $g_{MN}(\mu,\nu)$, which in the transfer matrix formalism becomes

$$g_{MN}(\mu,\nu)=\text{tr}\,(\sigma^x_{m+\mu M}V^{\nu N}\sigma^x_m V^{(1-\nu)N})/\text{tr}\,V^N. \tag{5.20}$$

We assume $T<T_c$, so that the two largest eigenvalues of V are degenerate (more precisely, they differ by $O(e^{-M})$ for large M; such differences are consistently neglected). For $T>T_c$ there is no degeneracy so all proofs are similar but simpler.

The denominator of (5.20) can be accurately bounded because $\epsilon_q \geq \epsilon_{\min}>0$ for all $q\neq 0$:

$$2\Lambda_0^N<\text{tr}\,V^N<2\Lambda_0^N[1+\exp(-N\epsilon_{\min})]^{M-1}<2\Lambda_0^N \times\exp[(M-1)\exp(-N\epsilon_{\min})].$$

For large M and N, then, with negligible error,

$$\text{tr}\,V^N=2\Lambda_0^N, \tag{5.21}$$

i.e., the sole contribution when N and M are large comes from the two maximum eigenvalues of V.

If we expand the numerator of (5.20) in the eigenvectors of V we have

$$g_{MN}(\mu,\nu)=\tfrac{1}{2}\sum_{\alpha,\beta}\langle\Psi_\alpha\,|\,\sigma^x_{m+\mu M}\,|\,\Psi_\beta\rangle\langle\Psi_\beta\,|\,\sigma^x_m\,|\,\Psi_\alpha\rangle\left(\frac{\Lambda_\alpha}{\Lambda_0}\right)^{(1-\nu)N}\left(\frac{\Lambda_\beta}{\Lambda_0}\right)^{\nu N}. \tag{5.22}$$

We have suppressed the subscript M on all matrix elements and eigenvalues. Let us separate explicitly terms in which one or both eigenvectors belong to the maximum eigenvalue:

$$\begin{aligned}g_{MN}(\mu,\nu)=&\tfrac{1}{2}[\langle\Psi^+_0\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^-_{k=0}\rangle\langle\Psi^-_{k=0}\,|\,\sigma^x_m\,|\,\Psi^+_0\rangle+\text{c.c.}]\\&+\tfrac{1}{2}\Big[\sum_{\beta\gtrless(k=0)}\langle\Psi^+_0\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^-_\beta\rangle\langle\Psi^-_\beta\,|\,\sigma^x_m\,|\,\Psi^+_0\rangle\left(\frac{\Lambda_\beta}{\Lambda_0}\right)^{\nu N}+\sum_{\beta\neq 0}\langle\Psi^-_{k=0}\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^+_\beta\rangle\langle\Psi^+_\beta\,|\,\sigma^x_m\,|\,\Psi^-_{k=0}\rangle\left(\frac{\Lambda_\beta}{\Lambda_0}\right)^{\nu N}\Big]\\&+\tfrac{1}{2}\Big[\sum_{\alpha\gtrless(k=0)}\langle\Psi^-_\alpha\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^+_0\rangle\langle\Psi^+_0\,|\,\sigma^x_m\,|\,\Psi^-_\alpha\rangle\left(\frac{\Lambda_\alpha}{\Lambda_0}\right)^{(1-\nu)N}+\sum_{\alpha\neq 0}\langle\Psi^+_\alpha\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^-_{k=0}\rangle\langle\Psi^-_{k=0}\,|\,\sigma^x_m\,|\,\Psi^+_\alpha\rangle\left(\frac{\Lambda_\alpha}{\Lambda_0}\right)^{(1-\nu)N}\Big]\\&+\tfrac{1}{2}\Big[\sum_{\substack{\alpha\gtrless 0,(k=0)\\ \beta\gtrless 0,(k=0)}}\langle\Psi_\alpha\,|\,\sigma^x_{m+\mu M}\,|\,\Psi_\beta\rangle\langle\Psi_\beta\,|\,\sigma^x_m\,|\,\Psi_\alpha\rangle\left(\frac{\Lambda_\alpha}{\Lambda_0}\right)^{(1-\nu)N}\left(\frac{\Lambda_\beta}{\Lambda_0}\right)^{\nu N}\Big].\end{aligned} \tag{5.23}$$

We have explicitly recognized the fact that operators like $\sigma^x_{m+\mu M}$ and σ^x_m only connect states of odd numbers of fermions with states of even numbers.

We now wish to show that, when $M, N\to\infty$, $g_{MN}(\mu,\nu)$ is approximated with arbitrary accuracy by the first bracket on the right. It may be remarked that this first bracket can be simplified because

$$\langle\Psi^-_{k=0}\,|\,\sigma^x_m\,|\,\Psi^+_0\rangle=\langle\Psi^-_{k=0}\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^+_0\rangle$$

by translational invariance, so the two terms within the bracket are the same.

Using Schwarz's inequality, the first term in the second bracket is bounded in absolute value by

$$\exp(-\nu N\epsilon_{\min})[\sum_{\beta\gtrless(k=0)}|\,\langle\Psi^+_0\,|\,\sigma^x_{m+\mu M}\,|\,\Psi^-_\beta\rangle\,|^2]^{\frac{1}{2}} \times[\sum_{\beta\gtrless(k=0)}|\,\langle\Psi^-_\beta\,|\,\sigma^x_m\,|\,\Psi^+_0\rangle\,|^2]^{\frac{1}{2}}. \tag{5.24}$$

If we include the term with $\beta=(k=0)$ in the sums and use the fact that $(\sigma^x_m)^2=1$, etc. this is in turn bounded by $\exp(-\nu N\epsilon_{\min})$. Similar arguments hold for the other term in the second bracket and both terms in the third bracket. The fourth bracket is similarly bounded, in absolute value, by $2^M\exp(-N\epsilon_{\min})$. Thus

$$|\,g_{MN}(\mu,\nu)-|\,\langle\Psi^+_0\,|\,\sigma^x_m\,|\,\Psi^-_{k=0}\rangle_M\,|^2|\leq\exp(-\nu N\epsilon_{\min}) +\exp[-(1-\nu)N\epsilon_{\min}]+2^M\exp(-N\epsilon_{\min}). \tag{5.25}$$

And so, taking the limit $N, M\to\infty$,

$$g(\mu,\nu)\equiv\lim_{M,N\to\infty}|\,\langle\Psi^+_0\,|\,\sigma^x_m\,|\,\Psi^-_{k=0}\rangle_M\,|^2\equiv g, \qquad \nu>0. \tag{5.26}$$

A similar argument with the transfer matrix going from column to column shows that $g(\mu,\nu)$ is a constant, but restricted only by the requirement $\mu>0$. Thus (5.26) holds on both the μ and ν axes as well as in the quadrant $\mu>0$, $\nu>0$ and

$$|\,\mathfrak{M}_s\,|=\lim_{M\to\infty}|\,\langle\Psi^+_0\,|\,\sigma^x_m\,|\,\Psi^-_{k=0}\rangle_M\,|. \tag{5.27}$$

[32] Strictly speaking (5.15) is $\mathfrak{M}_s^2=\lim_{M,N\to\infty}(MN)^{-1}\sum_{x,y}g_{MN}(\mu,\nu)$ with x and y ranging over a quasicontinuous mesh. The replacement of the Riemann sum of the function $g_{MN}(\mu,\nu)$ by the Riemann integral of the limit function $g(\mu,\nu)$ can be justified because of the exponentially rapid convergence of the $g_{MN}(\mu,\nu)$ to $g(\mu,\nu)$.

It is this form of (5.15), essentially, from which Yang computed the spontaneous magnetization.

Having proved that the long long-range order is a constant, independent of direction of separation of the two sites, we now observe that this is also true for the short long-range order and in fact the two are the same. We have only to point out that in deriving (5.26) we required only that $\nu N\to\infty$, i.e., that $n'-n\to\infty$, and not that ν remain fixed. Thus $f(\alpha)\equiv g$ for all α, and we have a second equivalent form for the spontaneous magnetization obtained from the short long-range order in a row, the form used by MPW:

$$\mathfrak{M}_s=[\lim_{m'-m\to\infty}\lim_{M,N\to\infty}\langle\sigma^x_{m'}\sigma^x_m\rangle_{MN}]^{\frac{1}{2}}$$
$$=\left[1-\frac{(1-\tanh^2 K_1)^2(1-\tanh^2 K_2)^2}{16\tanh^2 K_1\tanh^2 K_2}\right]^{1/8}. \quad (5.28)$$

We remark that for $T>T_c$ there is only one eigenvector of maximum eigenvalue. There is therefore no term corresponding to the first bracket in (5.23); and so, $g(x,y)\equiv f(\alpha)\equiv 0$, and $\mathfrak{M}_s=0$.

C. Yang's Approach to Spontaneous Magnetization

We now consider Yang's derivation of the spontaneous magnetization to make explicit the implicit assumption that $\mathfrak{H}=O(1/M)$. Yang observed that if the spontaneous magnetization is to be nonvanishing, the partition function and therefore the largest eigenvalue of the transfer matrix must have a first-order contribution from $\mathfrak{H}$ or H. Let us then first derive the expansion of the transfer matrix to this order. Recalling that V_2 and V_3 commute, we can write

$$V(H)=V_3^{\frac{1}{2}}VV_3^{\frac{1}{2}}, \quad (5.29)$$

where by V we mean the transfer matrix in the absence of a magnetic field. Expanding $V_3^{\frac{1}{2}}$,

$$V_3^{\frac{1}{2}}=1+\tfrac{1}{2}H\sum\sigma^x_m+\cdots \quad (5.30)$$

we obtain a formal expansion for $V(H)$:

$$V(H)=V+\tfrac{1}{2}H\{\sum\sigma^x_m, V\}+\cdots. \quad (5.31)$$

We can already see that because $\sum\sigma^x_m$ is an operator whose eigenvalues are of order M, the second term is of order HM times the first term. For H larger than $O(1/M)$ it would be essential to include terms of all orders and hope that the correction to the eigenvalue of V could in some sense be exponentiated (as is almost always the case in many-body theory), i.e., we would expect $\Lambda_0(H)$ to be of the form

$$\Lambda_0(H)=\Lambda_0\exp(b_1|H|+b_2H^2+\cdots)$$

where b_1, b_2, etc. are constants of order M. Since we must content ourselves with the expansion (5.31), we assume that $H=\alpha/M$ and that α ultimately tends to zero. At best only b_1 is then obtained.

We now observe that the diagonal matrix elements of the term in (5.31) that is linear in H, for the eigenvectors of V, all vanish. Thus for $T>T_c$, when the largest eigenvector is nondegenerate, there is no modification of Λ_0 or the free energy to first order in H and so $\mathfrak{M}_s=0$. Below the transition temperature, when the largest eigenvectors are exponentially degenerate, in the limit $M\to\infty$, there is a first-order effect obtained by diagonalizing $V(H)$ between the two maximum eigenvectors. The matrix of $V(H)$, in this limit is

$$V(H)\simeq\begin{pmatrix}\Lambda_0 & \Lambda_0H\langle\Psi^+_0|\sum\sigma^x_m|\Psi^-_{k=0}\rangle\\ \Lambda_0H\langle\Psi^+_0|\sum\sigma^x_m|\Psi^-_{k=0}\rangle^* & \Lambda_0\end{pmatrix} \quad (5.32)$$

and the maximum eigenvalue [belonging to the vector $2^{-\frac{1}{2}}(\Psi^+_0+\Psi^-_{k=0})$] is

$$\Lambda_0(H)\simeq\Lambda_0(1+|H||\langle\Psi^+_0|\sum\sigma^x_m|\Psi^-_{k=0}\rangle|)$$
$$\simeq\Lambda_0\exp(|H||\langle\Psi^+_0|\sum\sigma^x_m|\Psi^-_{k=0}\rangle|), \quad (5.33)$$

from which one derives essentially Yang's expression[33] for the spontaneous magnetization,

$$\mathfrak{M}_s=\lim_{M\to\infty}|\langle\Psi^+_0|M^{-1}\sum_m\sigma^x_m|\Psi^-_{k=0}\rangle_M|. \quad (5.34)$$

[33] Yang's expression actually reduces to

$$\Lambda_0\exp(|H||\langle\Psi_0'|\Sigma\sigma^x_m|\Psi_{k=0}'\rangle|\cosh 2K_1^*),$$

where Ψ_0' and $\Psi_{k=0}'$ are vectors defined for the transfer matrix $V'=V_1^{\frac{1}{2}}V_2V_1^{\frac{1}{2}}$ rather than for $V=V_2^{\frac{1}{2}}V_1V_2^{\frac{1}{2}}$ as presented here.

For cyclic boundary conditions in the rows, the matrix element $\langle \Psi^+_0 \mid \sigma^x_m \mid \Psi^-_{k=0} \rangle$ is strictly independent of m so that (5.34) reduces to

$$\mathfrak{M}_s = \lim_{M\to\infty} \mid \langle \Psi^+_0 \mid \sigma^x_1 \mid \Psi^-_{k=0} \rangle_M \mid \qquad (5.34')$$

agreeing with (5.27).[34]

It is an easy matter to express $\sigma^x_1 = C_1^\dagger + C_1$ in terms of the ξ_l's and $\xi_l^\dagger$'s or in terms of the ξ_k's and $\xi_k^\dagger$'s. The difficulty in evaluating $\langle \Psi^+_0 \mid \sigma^x_1 \mid \Psi^-_{k=0} \rangle$ is that Ψ^+_0 is the Fermi vacuum for the ξ_l particles, while $\Psi^-_{k=0}$ is obtained from the Fermi vacuum for the ξ_k particles. The two vacuum states Ψ^+_0 and Ψ^-_0 are not simply related. This difficulty can be circumvented if one introduces free-end boundary conditions. There is then only one Fermi vacuum, and the second-degenerate state is a simple single-excitation state from that vacuum. Now, however, the translational degeneracy is lost and one must consider the matrix element of σ^x_m, $m \gg 1$, not just of σ^x_1.

[34] The condition that $H = \alpha/M$, $\alpha \to 0$, which is required for the exponentiation of (5.33a) to obtain (5.33b), seems unnecessarily restrictive. One wonders if higher terms in the series (5.33a) confirm the exponential form (5.33b). For example, to calculate the H^2 term in $\Lambda_0(H)$, we observe that the H^2 term in the formal expansion (5.31) is

$$\tfrac{1}{2}H^2 \sum_{mm'} (\sigma^x_m V \sigma^x_{m'} + \tfrac{1}{2}\{\sigma^x_m \sigma^x_{m'}, V\}).$$

The H^2 term in the expansion of $\Lambda_0(H)$ has two contributions, the diagonal contribution of this second-order term from the eigenvector $2^{-\frac{1}{2}}(\Psi^+_0 + \Psi^-_{k=0})$, and the second-order perturbation theoretic contribution from $\frac{1}{2}H\{\Sigma\sigma^x_m, V\}$. Straightforward calculation gives, to order H^2

$$\Lambda_0(H) = \Lambda_0[1 + \mid H \mid \langle \Psi^+_0 \mid \sum_m \sigma^x_m \mid \Psi^-_{k=0} \rangle + \tfrac{1}{2}H^2 \langle \Psi^+_0 \mid \sum_{mm'} \sigma^x_m \sigma^x_{m'} \mid \Psi^+_0 \rangle + H^2 \sum_\alpha{}' \Lambda_\alpha (\Lambda_0 - \Lambda_\alpha)^{-1} \mid \langle 2^{-\frac{1}{2}}(\Psi^+_0 + \Psi^-_{k=0}) \mid \Sigma\sigma^x_m \mid \Psi_\alpha \rangle \mid^2],$$

where we have used the facts that $\langle \Psi^+_0 \mid \sigma^x_m \mid \Psi^-_{k=0} \rangle$ is real and that $\langle \Psi^+_0 \mid \Sigma\sigma^x_m \sigma^x_{m'} \mid \Psi^+_0 \rangle = \langle \Psi^-_{k=0} \mid \Sigma\sigma^x_m \sigma^x_{m'} \mid \Psi^-_{k=0} \rangle$. In the last term, the set of $\{\Psi_\alpha\}$ includes all allowable eigenvectors of V but the two maximum ones.

We observe first that, because of (5.26), the first three terms are, to within corrections terms of order H^2M, precisely what one would obtain if $\Lambda_0(H)$ had the form $\exp(\mid H \mid \langle \Psi^+_0 \mid \Sigma\sigma^x_m \mid \Psi^-_{k=0} \rangle)$. For the last term, because $\Lambda_\alpha < \Lambda_0$, one can obtain the upper bound

$$(\Lambda_0/\Lambda_1 - 1)^{-1} H^2 \{ \langle \Psi^+_0 \mid (\Sigma\sigma^x_m)^2 \mid \Psi^+_0 \rangle - \mid \langle \Psi^+_0 \mid \sigma^x_m \mid \Psi^-_{k=0} \rangle \mid^2 \} = O(H^2 M).$$

Thus the asymptotic equality (5.26) is sufficient to verify the exponential form of $\Lambda_0(H)$ up to second order in H when $M \to \infty$. More detailed analysis shows that this holds for terms of higher order in H until terms of order $H^{O(M)}$. This is precisely analogous to the problem of proving the sufficient sharpness of $p_{MN}(\mathfrak{M})$ through analysis of its very high moments.

VI. SUMMARY

In this paper we have tried to reduce the algebraic solution of the Ising model on a square lattice to a sequence of simple steps, so that the whole solution, originally considered so complex and obscure, would be transparent and not require knowledge of special algebraic techniques. It might be useful in conclusion to summarize these steps.

First we introduced the transfer matrix, which relates the density operator of the last row in an N-row lattice to that for an $(N-1)$-row lattice and expressed this matrix in terms of the spin operators for the last row. This step is not limited to the two-dimensional problem (for three dimensions, the "last row" becomes the last plane).

Second, we transformed the spin operators in that row to fermion annihilation and creation operators. Such a transformation is always possible when the spins can be numbered in some order, although the transformed operators are convenient when only nearest neighbors in the ordering interact (thus limiting the method to two dimensions) and when the operators of interest are all bilinear in spin raising and lower operators (thus limiting the method to vanishing magnetic field).

Third, we introduced running-wave fermion operators, made possible by cyclic boundary conditions. The transfer operator is then a product of commuting operators each of which involves simple quadratic forms of the paired type, similar to what occurs in the BCS theory of superconductivity.

Fourth, we diagonalized the transfer matrix by a Bogolubov–Valatin transformation. The complications introduced by using periodic boundary conditions were not fundamental and only required more careful bookkeeping.

Fifth, we used Wick's theorem to show that the correlation function between two spins in the same row is a determinant, and we showed the relation to the results previously obtained in the literature.

Finally, we have analyzed the problem of spontaneous magnetization, pointing out the discrepancies between the correct definition of spontaneous magnetization and those previously used. In the course of this analysis we have shown rigorously that what we have called the *long* and *short* long-range orders are equal and independent of direction.

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Solution of the Dimer Problem by the Transfer Matrix Method

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It is shown how the monomer–dimer problem can be formulated in terms of a transfer matrix, and hence in terms of simple spin operators as was originally done for the Ising problem. Thus, we rederive the solution to the pure dimer problem without using Pfaffians. The solution is extremely simple once one sees how to formulate the transfer matrix.

1. INTRODUCTION

SINCE Onsager's solution[1] of the two-dimensional Ising model in 1944, there has been a great deal of activity in the general area of nearest neighbor planar lattice problems. Basically, two approaches have been used.[2] One is the "algebraic" or "transfer matrix" method (used by Onsager) which focuses attention on the manner in which two neighboring rows are connected to each other. The second is the so-called "combinatorial method" whereby one studies graphs on the lattice as a whole. This was first used by Kac and Ward[3] for the Ising problem.

The most recent and concise formulation of the combinatorial method reduces the various problems to the evaluation of a Pfaffian. This method had its first "original" success in the solution to the dimer problem by Kasteleyn,[4] and for this reason is also referred to as the dimer method.

While Pfaffians have been used to rederive the solution to the Ising problem,[5] no one has yet taken the complementary step of solving the dimer problem by the transfer matrix method. The purpose of this note is to eliminate this gap. Elsewhere,[6] it has been shown how the transfer matrix method for Ising-like problems can be reduced to a few simple steps involving only fermion creation and annihilation operators. The dimer problem is likewise simple, using the transfer matrix. We also show how the more difficult and unsolved monomer–dimer problem can be formulated this way. The analogy with the problem of the Ising model in a magnetic field is very transparent, but the monomer–dimer problem is somewhat simpler and therefore there is considerable hope that this new formulation of the problem may ultimately lead to its solution.

2. FORMULATION OF THE TRANSFER MATRIX

We have a square planar lattice of M rows and N columns and hence MN vertices. A dimer is a rigid rod just long enough to cover two neighboring

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vertices (either horizontally or vertically), while a monomer covers just one vertex. An allowed configuration of the lattice is one in which every vertex is covered by a monomer or a dimer such that no vertex is covered by more than one object. If h, v, and m, are, respectively, the numbers of horizontal dimers, vertical dimers, and monomers in a configuration (with $2h + 2v + m = MN$), then the partition function Z is

$$\begin{aligned} Z &= \sum \begin{pmatrix} \text{ALLOWED} \\ \text{CONFIGURATIONS} \end{pmatrix} x^h y^v z^m \\ &= y^{\frac{1}{2}MN} \sum \begin{pmatrix} \text{ALLOWED} \\ \text{CONFIGURATIONS} \end{pmatrix} \alpha^h \beta^m \end{aligned} \tag{2.1}$$

where x, y, and z are the appropriate "activities" and $\alpha = x/y$, $\beta = z/(y)^{\frac{1}{2}}$.

Beginning at the "bottom" of the lattice, we have a row of N vertical bonds (V bonds) followed by a row of N horizontal bonds (H bonds), and so on alternately. There are M bond rows of each type. On each V bond of the first row, we place an arrow (or spin): an up arrow (spin +) signifies the presence of a vertical dimer on that bond, while a down arrow (spin −) signifies the absence of a dimer. The next row consists of NH bonds alternating with N vertices. If an arrow points into one of these vertices (i.e., spin + on the previous V bond) that vertex is saturated and only a down arrow must be allowed to propagate out of that vertex along the next V bond. If, however, a down arrow (spin −) comes into a vertex from below, one of three things are allowed to happen: (1) an up arrow (= dimer = spin +) can propagate along the next V bond; (2) two neighboring down arrows can cooperate to form a horizontal dimer on the intervening H bond, which means that down arrows must propagate upwards from those two vertices; (3) a down arrow can propagate upwards from the vertex in question, signifying that a monomer has been placed on that vertex.

These rules seem complicated but they can be simply formulated if one decomposes the activity on the row of vertices into two simple steps.

Step 1: Reverse all the incoming arrows. The operator that accomplishes this is simply

$$V_1 = \prod_{i=1}^{N} \sigma_i^x, \tag{2.2}$$

where σ^x is the Pauli spin matrix $\sigma^x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. The operator V_1 guarantees that an incoming up arrow (spin +) will go out as a down arrow, as required. Contrariwise, an incoming down arrow (no dimer) will propagate upwards as a V dimer (spin +). To create monomers or H dimers on the row of H bonds under consideration, it is necessary to convert some of these up arrows to down arrows and this is accomplished by the second step.

Step 2: To create a monomer at the jth vertex of the row, we multiply by σ_j^-, where $\sigma^- = \left(\begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix}\right)$. To create a horizontal dimer at the adjacent sites j and $j + 1$, we multiply by $\sigma_j^- \sigma_{j+1}^-$. Note that after multiplication by these operators, we are insured that only down arrows (i.e., no vertical dimers) propagate onto the next row of V bonds.

The operator which generates exactly m monomers on the row is $(m!)^{-1}(\sum_{i=1}^{N} \sigma_i^-)^m$ because $(\sigma_i^-)^2 = 0$. Thus, to generate an arbitrary number of monomers with the factor β^m, we multiply by the operator

$$V_2 = \exp\left(\beta \sum_{i=1}^{N} \sigma_i^-\right). \tag{2.3}$$

Likewise, to generate H dimers, we multiply by

$$V_3 = \exp\left(\alpha \sum_{i=1}^{N} \sigma_i^- \sigma_{i+1}^-\right). \tag{2.4}$$

In Eq. (2.4), we have used cyclic boundary conditions with $\sigma_{N+1}^- \equiv \sigma_1^-$. If free ends are desired, then omit the term $\sigma_1^- \sigma_N^-$.

Thus, our transfer matrix is

$$V = V_3 V_2 V_1, \tag{2.5}$$

and

$$Z = y^{\frac{1}{2}MN} \operatorname{Tr} V^M, \tag{2.6}$$

where we have used cyclic boundary conditions in the vertical direction. We note that free edge (noncyclic) boundary conditions can be used in either or both directions with no great complication, although we shall confine ourselves here to cyclic boundary conditions.

The problem is thus reduced to computing the eigenvalues of V.

3. DIAGONALIZATION OF THE TRANSFER MATRIX

It is convenient, although not essential, to eliminate V_1. To do so, we consider $V^2 = V_3 V_2 V_1 V_3 V_2 V_1$ and make use of the fact that σ_i^x is a unitary operator with $\sigma_i^x \sigma_i^- \sigma_i^x = \sigma_i^+ = \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$. Thus,

$$V^2 = V_3 V_2 \bar{V}_3 \bar{V}_2 \tag{3.1}$$

with

$$\begin{aligned} \bar{V}_2 &= \exp\left(\beta \sum_{i=1}^{N} \sigma_i^+\right), \\ \bar{V}_3 &= \exp\left(\alpha \sum_{i=1}^{N} \sigma_i^+ \sigma_{i+1}^+\right). \end{aligned} \tag{3.2}$$

Thus,

$$Z = y^{\frac{1}{2}MN} \sum_j \lambda_j(N)^{\frac{1}{2}M}, \tag{3.3}$$

where $\lambda_j(N)$ (for $j = 1, 2, \cdots, 2^N$) are the eigenvalues of V^2 (we have assumed M is even).

The operator V contains two kinds of operators: quadratic forms (as in V_3 and $\bar{V}_3$) and linear forms (as in V_2 and $\bar{V}_2$). It is similar to, but simpler than, the problem of the Ising model in a magnetic field, because V_2 and V_3 commute and because V_2 is the adjoint of $\bar{V}_2$ and V_3 is the adjoint of $\bar{V}_3$. Nevertheless, we still are unable to handle the linear forms and henceforth we shall set $\beta = 0$ (i.e., we consider only the pure dimer problem).

The appropriate steps to diagonalize $V_3\bar{V}_3$ are well known. The details are in Ref. 6 and it suffices to outline the steps here. First, we transform from paulions to fermions:

$$\begin{aligned} C_j &\equiv (-1)^{j-1}\left(\prod_{i=1}^{j-1}\sigma_i^z\right)\sigma_j^-, \\ C_j^\dagger &\equiv (-1)^{j-1}\left(\prod_{i=1}^{j-1}\sigma_i^z\right)\sigma_j^+, \end{aligned} \tag{3.4}$$

with $\sigma^z = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$.

This results in

$$\begin{aligned} \sigma_j^-\sigma_{j+1}^- &= -C_jC_{j+1}, \\ \sigma_j^+\sigma_{j+1}^+ &= C_j^\dagger C_{j+1}^\dagger, \end{aligned} \tag{3.5}$$

while

$$\begin{aligned} \sigma_1^-\sigma_N^- &= (-1)^{\mathcal{N}}C_NC_1, \\ \sigma_1^+\sigma_N^+ &= -(-1)^{\mathcal{N}}C_N^\dagger C_1^\dagger, \end{aligned} \tag{3.6}$$

where $\mathcal{N} = \sum_1^N C_i^\dagger C_i$ is the number operator.

Since $(-1)^{\mathcal{N}}$ commutes with a quadratic form in fermions (or paulions), it is a constant of the motion $= +1$ for states of even $\mathcal{N}$ and -1 for states of odd $\mathcal{N}$. The latter case is cyclic while the former is anticyclic.

Next we go to running waves:

$$C_j = N^{-\frac{1}{2}}e^{-i\pi/4}\sum_q e^{iqj}\eta_q, \tag{3.7}$$

with

$$q = \pm\pi/N, \pm 3\pi/N, \cdots, \pm(N-1)\pi/N \tag{3.8a}$$

for $\mathcal{N}$ even, and

$$q = 0, \pm 2\pi/N, \pm 4\pi/N, \cdots, \pm(N-2)\pi/N, \pi \tag{3.8b}$$

for $\mathcal{N}$ odd. (We have assumed that N is even.) In terms of these running waves, we have

$$V^2 = \prod_{0\le q\le\pi} A_q \tag{3.9}$$

with

$$A_q = \exp(2\alpha \sin q\eta_q\eta_{-q}) \exp(2\alpha \sin q\eta_{-q}^\dagger\eta_q^\dagger). \tag{3.10}$$

Obviously, A_q and $A_{q'}$ commute with each other. An eigenvalue of V^2 is thus the product of eigenvalues of each A_q, but we must remember to use the appropriate q values [(3.8a) or (3.8b)] according to whether the total $\mathcal{N}$ value of a state is even or odd.

To diagonalize A_q (for $q \neq 0$ and $q \neq \pi$), we first list the four basis states,

$$\begin{aligned} &\Phi_0 = |0\rangle, \quad \Phi_q = \eta_q^\dagger|0\rangle, \quad \Phi_{-q} = \eta_{-q}^\dagger|0\rangle, \\ &\Phi_{-qq} = \eta_{-q}^\dagger\eta_q^\dagger|0\rangle. \end{aligned} \tag{3.11}$$

The states Φ_q and Φ_{-q} are pure odd states and are eigenvectors of A_q with eigenvalue unity. The other two states are pure even and

$$\begin{aligned} A_q\Phi_0 &= (1 + 4\alpha^2\sin^2 q)\Phi_0 + 2\alpha \sin q\Phi_{-qq}, \\ A_q\Phi_{-qq} &= 2\alpha \sin q\Phi_0 + \Phi_{-qq}. \end{aligned} \tag{3.12}$$

The two even eigenvalues of A_q are thus

$$\lambda_{\text{even}} = [\alpha \sin q \pm (1 + \alpha^2 \sin^2 q)^{\frac{1}{2}}]^2. \tag{3.13}$$

For $q = 0$ or π there are only two states: $\Phi_0 = |0\rangle$ (even) and $\Phi_q = \eta_q^\dagger|0\rangle$ (odd). Both have eigenvalue unity. These values of q are effective only for $\mathcal{N}$ odd and these pairs of states may be used to insure that $\mathcal{N}$ is always odd without affecting the total eigenvalue.

Thus, from (3.3),

$$\begin{aligned} y^{-\frac{1}{2}MN}Z = 2 &\prod_{\substack{0<q<\pi \\ q\in(3.8b)}} \{[(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} + \alpha \sin q]^M \\ &+ [(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} - \alpha \sin q]^M + (1 + 1)\} \\ &+ \tfrac{1}{2}\prod_{\substack{0<q<\pi \\ q\in(3.8a)}} \{[(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} + \alpha \sin q]^M \\ &+ [(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} - \alpha \sin q]^M + (1 + 1)\} \\ &+ \tfrac{1}{2}\prod_{\substack{0<q<\pi \\ q\in(3.8a)}} \{[(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} + \alpha \sin q]^M \\ &+ [(1 + \alpha^2\sin^2 q)^{\frac{1}{2}} - \alpha \sin q]^M - (1 + 1)\}. \end{aligned} \tag{3.14}$$

The first product in (3.14) gives the contribution of the $\mathcal{N}$ odd eigenvalues while the sum of the second and third products gives the contribution of the $\mathcal{N}$ even eigenvalues. [Eq. (3.14) agrees exactly with Kasteleyn's result (Ref. 4, Eq. (25)), as may be seen using Kasteleyn's identity (Ref. 4, Eq. (26)).]

For a large lattice ($MN \to \infty$), we need consider only the largest eigenvalue of V^2, which means the product on all q of Eq. (3.13), using the plus sign. In this limit, it clearly is immaterial which set we use, (3.8a) or (3.8b). Thus,

$$\begin{aligned} &\lim_{M,N\to\infty} (MN)^{-1} \ln Z \\ &\quad = \frac{1}{2\pi}\int_0^\pi dq \ln[\alpha \sin q + (1 + \alpha^2 \sin^2 q)^{\frac{1}{2}}] \\ &\qquad + \tfrac{1}{2}\ln y, \end{aligned} \tag{3.15}$$

which agrees with previous results[4] for the pure dimer problem.

Part XI

Spin Chains

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Two Soluble Models of an Antiferromagnetic Chain

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Two genuinely quantum mechanical models for an antiferromagnetic linear chain with nearest neighbor interactions are constructed and solved exactly, in the sense that the ground state, all the elementary excitations and the free energy are found. A general formalism for calculating the instantaneous correlation between any two spins is developed and applied to the investigation of short- and long-range order. Both models show nonvanishing long-range order in the ground state for a range of values of a certain parameter λ which is analogous to an anisotropy parameter in the Heisenberg model. A detailed comparison with the Heisenberg model suggests that the latter has no long-range order in the isotropic case but finite long-range order for any finite amount of anisotropy. The unreliability of variational methods for determining long-range order is emphasized. It is also shown that for spin $\frac{1}{2}$ systems having rather general isotropic Heisenberg interactions favoring an antiferromagnetic ordering, the ground state is nondegenerate and there is no energy gap above the ground state in the energy spectrum of the total system.

I. INTRODUCTION

For an infinite chain of spins interacting with nearest neighbors via a Heisenberg interaction, the exact energy eigenstates were found, in principle, many years ago by Bethe (*1*) and the ground-state energy was found somewhat later by Hulthén (*2*). The problem has nevertheless occasioned a persistent theoretical interest. This is because the exact method of Bethe does not seem capable of generalization to the more interesting cases of two and three dimensions. The aim has generally been to construct approximate methods that give accurate results in one dimension, as determined by a comparison with the known exact results, but which can be generalized to two or three dimensions with some degree of confidence and simplicity. Unfortunately, the crucial test for any approximate method is how well it describes the long-range order; but it is precisely this test which has been impossible, because the long-range order has never been calculated exactly by the method of Bethe.

There is, in fact, still considerable doubt about the nature of the long-range order in one or more dimensions. On the one hand, spin wave methods used by Anderson (*3*) and Kubo (*4*) have predicted long-range order in two or three dimensions, although Anderson (but not Kubo) predicts no long-range order in one dimension. Variational methods of Kasteleijn (*5*) generalized to two and

three dimensions by Taketa and Nakamura (*6*), and of Marshall (*7*), all related to a variational method of Hulthén (*2*), indicate no long-range order in one, two, and three dimensions for the completely isotropic interaction. On the other hand, they all predict the onset of long-range order for a certain critical amount of anisotropy—the same amount at which a kink is predicted for the short-range order. Exact calculations by Orbach (*8*) on the anisotropic case, generalizing the method of Bethe, show the kink to be spurious for the one-dimensional case, but throw no further light on the long-range order. Walker (*9*) has observed that the ground-state energy calculated by Orbach has a power series expansion around the limiting case of the completely anisotropic interaction (Ising limit) which seems to give a good representation of the ground-state energy even for the isotropic case, although he observes that a similar expansion for the long-range order suggests the long-range order might vanish when the anisotropy falls below a certain critical value. Ruijgrok and Rodriguez (*10*) have developed a variational method for the one-dimensional case which gives a good value for the ground-state energy, significantly better than previous variational methods, and which also predicts finite long-range order. Davis (*11*) has performed a perturbation theoretic calculation which indicates, to the order to which it has been carried, a long-range order in any number of dimensions even for the isotropic case.

There are two questions raised by all these investigations. First, can a purely isotropic Heisenberg interaction between nearest neighbors produce long-range order in any number of dimensions? Second, if such an ordering tendency exists in, say, two or three dimensions, will it also exist in only one dimension, or would the absence of order in one dimension prove nothing at all about order in two or three dimensions?

The purpose of the present paper is to gain further insight into the effects of anisotropy in one dimension. Two models will be constructed which can be solved exactly in considerable detail and which bear a reasonably close resemblance to the Heisenberg model. The investigation of the first of these models strongly suggests that the isotropic Heisenberg model has no long-range order but that such order exists for any finite amount of anisotropy. Both models emphasize the subtle nature of long-range order and the insufficiency of variational methods as a reliable approach to this question. The question of the relation of these results to two- and three-dimensional cases is left completely open.

In Section II we consider the first of these models, the "XY model." It is shown that the Hamiltonian can be expressed as a quadratic form in creation and annihilation operators for fermions, and this quadratic form can be diagonalized, thereby giving the complete set of states, excitation energies, and partition sum. In terms of these operators, general expressions for the order between any two spins are derived involving a kind of Green function, G_{ij}, which can be explicitly

evaluated. The general relation between the order and G_{ij} is equally valid for the Heisenberg model, but G_{ij} itself is then not explicitly calculable. The short-, intermediate-, and long-range order are calculated for various situations, and it is shown that only for the isotropic case does the long-range order vanish. The model is compared with the Heisenberg model for one special case from which reasonable surmises may be made about the latter.

In Section III we consider the "Heisenberg-Ising model" in a similar way. Although the excited states and statistical mechanics are considerably more complicated, the conclusions about long-range order are much the same. An application of the method of Ruijgrok and Rodriguez to this model emphasizes the care with which one must interpret the results of variational calculations with regard to the ground-state energy.

II. THE XY MODEL

A. Formulation

The first model consists of N spin ½'s (N even) arranged in a row and having only nearest neighbor interactions. It is

$$H_\gamma = \sum_i [(1 + \gamma) S^x{}_i S^x{}_{i+1} + (1 - \gamma) S^y{}_i S^y{}_{i+1}], \tag{2.1}$$

where γ is a parameter characterizing the degree of anisotropy in the xy-plane. $S^x{}_i$, $S^y{}_i$ and $S^z{}_i$ may be represented by the usual Pauli spin matrices ($\hbar = 1$):

$$S^x{}_i = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad S^y{}_i = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \qquad S^z{}_i = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Because the Hamiltonian only involves the x- and y- components of the spin operators, we call this model the XY model.

The ends of the chain may be treated in at least two different but physically reasonable ways:

(i) as free ends, in which case the range of the summation index is $1 \leqq i \leqq N-1$, a situation that is convenient for discussing the long-range order;

(ii) as a cyclic chain, in which case $1 \leqq i \leqq N$ and $S^x{}_{N+1} \equiv S^x{}_1$, $S^y{}_{N+1} \equiv S^y{}_1$. This problem, or a slight variation of it (see below), is most convenient for for calculating interesting physical quantities other than the long-range order.

The XY model is exactly soluble for all values of γ, although we shall consider only the range $-1 \leqq \gamma \leqq 1$. Furthermore, it is strikingly similar to the generalized Heisenberg model described by the Hamiltonian

$$H_\gamma = \sum_i [(1 + \gamma) S^x{}_i S^x{}_{i+1} + (1 - \gamma)(S^y{}_i S^y{}_{i+1} + S^z{}_i S^z{}_{i+1})]. \tag{2.1'}$$

As $\gamma \to 1$ both models tend to the Ising model in which the x-components of spin are completely order and the y- and z-components are completely disordered. For $|\gamma| \neq 1$ both models are genuinely quantum mechanical because

different components of $\mathbf{S}_i$ appearing in H do not commute. The effect of the "transverse terms" (those multiplied by $1 - \gamma$ in either Hamiltonian) in both models is to oppose the ordering of the x-components but to favor the ordering of the y-components (and, in the Heisenberg model, of the z-components, too). Hitherto, it has not been clear for the Heisenberg model just how strong these two effects are: for any particular positive value of γ, do the transverse terms either establish any long-range order among the y- and z-components or destroy the long-range order of the x-components (which would imply absence of long-range order for the y- and z-components as well)? For the XY model, as we shall see, the transverse terms do neither until the limiting case $\gamma = 0$, when they succeed in destroying the order of the x-components. This result is highly suggestive for the Heisenberg model, a subject we discuss in detail in Section II F.

To solve the XY model, we first introduce the raising and lowering operators

$$a_i^\dagger = S^x{}_i + iS^y{}_i \quad \text{and} \quad a_i = S^x{}_i - iS^y{}_i \tag{2.2a}$$

in terms of which the Pauli spin operators are

$$S^x{}_i = (a_i^\dagger + a_i)/2; \qquad S^y{}_i = (a_i^\dagger - a_i)/2i; \qquad S^z{}_i = a_i^\dagger a_i - \tfrac{1}{2} \tag{2.2b}$$

and the Hamiltonian is

$$H_\gamma = \tfrac{1}{2}\sum_i [(a_i^\dagger a_{i+1} + \gamma a_i^\dagger a_{i+1}^\dagger) + \text{h.c.}]. \tag{2.3}$$

These operators partly resemble Fermi operators in that

$$\{a_i , a_i^\dagger\} = 1; \qquad a_i^2 = (a_i^\dagger)^2 = 0; \tag{2.4a}$$

and they partly resemble Bose operators in that

$$[a_i^\dagger, a_j] = [a_i^\dagger, a_j^\dagger] = [a_i , a_j] = 0, \qquad i \neq j. \tag{2.4b}$$

It is therefore not possible to diagonalize the quadratic form appearing in (2.3) directly with a canonical transformation; principal axis transformations of the a's and $a^\dagger$'s do not preserve this mixed set of canonical rules. However, it is possible to transform to a new set of variables that are strictly Fermi operators and in terms of which the Hamiltonian is just as simple.[1] Let

[1] This transformation from a set of Pauli spin operators to a set of fermion creation and annihilation operators dates back at least as far as the classical paper on second quantization of fermion fields by Jordan and Wigner (*12*). It is described in that context, for example, by Kramers (*12*). It was used as the basis for approximate calculations of the ground-state energy of the isotropic Heisenberg model independently by Meyer (*12*), and by Rodriguez (*12*). The more sophisticated variational calculation of an approximate ground-state energy and long-range order by Ruijgrok and Rodriguez (*10*) is also based on this transformation. A somewhat different procedure, based on the same idea of converting nearest neighbor pairs of "paulions" to nearest neighbor pairs of fermions, was applied to precisely $H_{\gamma=0}$ by Nambu (*12*). The spirit of our paper is, however, entirely different from the work of the previous

$$c_i \equiv \exp\left[\pi i \sum_1^{i-1} a_j^\dagger a_j\right] a_i \tag{2.5a}$$

and

$$c_i^\dagger \equiv a_i^\dagger \exp\left[-\pi i \sum_1^{i-1} a_j^\dagger a_j\right]. \tag{2.5b}$$

Then

$$c_i^\dagger c_i = a_i^\dagger a_i\,, \tag{2.6}$$

so that the inverse transformation is simply

$$a_i^\dagger = \exp\left[-\pi i \sum_1^{i-1} c_j^\dagger c_j\right] c_i\,, \tag{2.7a}$$

$$a_i^\dagger = c_i^\dagger \exp\left[\pi i \sum_1^{i-1} c_j^\dagger c_j\right]. \tag{2.7b}$$

The c's and $c^\dagger$'s are Fermi operators:

$$\{c_i\,, c_j^\dagger\} = \delta_{ij}\,, \tag{2.8a}$$

$$\{c_i\,, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0. \tag{2.8b}$$

Because $c_j^\dagger c_j$ is an occupation number having values 0 or 1,

$$\exp(\pi i c_j^\dagger c_j) = \exp(-\pi i c_j^\dagger c_j). \tag{2.9}$$

Furthermore, for $i = 1, 2, \ldots, N-1$,

$$a_i^\dagger a_{i+1} = c_i^\dagger c_{i+1} \tag{2.10a}$$

and

$$a_i^\dagger a_{i+1}^\dagger = c_i^\dagger c_{i+1}^\dagger, \tag{2.10b}$$

so that, for the case of free ends, the Hamiltonian is

$$H_\gamma = \tfrac{1}{2} \sum_1^{N-1} [(c_i^\dagger c_{i+1} + \gamma c_i^\dagger c_{i+1}^\dagger) + \text{h.c.}]. \tag{2.11}$$

For the cyclic chain, we need also

$$a_N^\dagger a_1 = -\, c_N^\dagger c_1 \exp\,(i\pi\mathfrak{N}) \neq c_N^\dagger c_1 \tag{2.12a}$$

and

$$a_N^\dagger a_1^\dagger = -\, c_N^\dagger c_1^\dagger \exp\,(i\pi\mathfrak{N}) \neq c_N^\dagger c_1^\dagger, \tag{2.12b}$$

authors, and the results are rather more extensive. Because the cases of particular interest ($\gamma \neq 0$, free ends) contain complications not previously encountered, we present here a detailed exposition of the mathematical tricks needed for the ultimate solution.

where

$$\mathfrak{N} \equiv \sum_1^N c_j^\dagger c_j = \sum_1^N (S^\gamma{}_j + \tfrac{1}{2}). \tag{2.13}$$

The Hamiltonian is

$$H_\gamma = \tfrac{1}{2} \sum_1^N [(c_i^\dagger c_{i+1} + \gamma c_i^\dagger c_{i+1}^\dagger) + \text{h.c.}] - \tfrac{1}{2}[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}] (\exp(i\pi\mathfrak{N}) + 1). \tag{2.11'}$$

That is, in terms of the Fermi operators c_i and $c_i^\dagger$, H_γ no longer has a simple cyclic structure. For large systems we may neglect the correction term proportional to $\exp(i\pi\mathfrak{N}) + 1$ in which case we call it the "c-cyclic" problem (the original problem being the "a-cyclic" problem). Actually it is not difficult to solve the a-cyclic problem exactly, but we shall first consider the simpler c-cyclic one.

In all cases, the Hamiltonian is a simple quadratic form in Fermi operators and can be exactly diagonalized. The particular simplicity of H_γ depends on the fact that the spins can be arranged in a definite order, that interactions occur only between neighboring spins in this ordering, and that the z-components of spin do not enter. If the interactions were to extend to nth nearest neighbors, H_γ would involve a polynomial of order $2n$ in the c's. In two-dimensional models, it can be readily seen that any ordering and nontrivial scheme of interactions must lead to a Hamiltonian involving a polynomial roughly of order $2N$ for a system of N^2 spins. Thus we are making maximum use of the nearest neighbor character of the interactions and the one-dimensionality of the system.

B. Ground-State Energy, Elementary Excitations, and Free Energy

The diagonalization of quadratic forms such as occur in (2.11) or (2.11') is discussed in Appendix A. The Hamiltonian is reduced to the diagonal form

$$H_\gamma = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \text{constant} \tag{2.14}$$

by the linear transformation

$$\eta_k = \sum_i \frac{\phi_{ki} + \psi_{ki}}{2} c_i + \frac{\phi_{ki} - \psi_{ki}}{2} c_i^\dagger, \tag{2.15a}$$

$$\eta_k^\dagger = \sum_i \frac{\phi_{ki} + \psi_{ki}}{2} c_i^\dagger + \frac{\phi_{ki} - \psi_{ki}}{2} c_i, \tag{2.15b}$$

where ϕ_k and ψ_k, considered as N-component vectors, are real solutions to certain matrix equations. For the c-cyclic problem, the relevant matrices

$$\mathbf{A} = \frac{1}{2}\begin{pmatrix} 0 & 1 & & & & & 1 \\ 1 & 0 & 1 & & & & \\ & \cdot & \cdot & \cdot & & \mathbf{0} & \\ & & \cdot & \cdot & \cdot & & \\ & \mathbf{0} & & \cdot & \cdot & \cdot & \\ & & & & 1 & 0 & 1 \\ 1 & & & & & 1 & 0 \end{pmatrix}, \tag{2.16a}$$

$$\mathbf{B} = \frac{1}{2}\gamma\begin{pmatrix} 0 & 1 & & & & & -1 \\ -1 & 0 & 1 & & & & \\ & \cdot & \cdot & \cdot & & \mathbf{0} & \\ & & \cdot & \cdot & \cdot & & \\ & \mathbf{0} & & \cdot & \cdot & \cdot & \\ & & & & -1 & 0 & 1 \\ 1 & & & & & -1 & 0 \end{pmatrix}, \tag{2.16b}$$

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) =$$

$$\frac{1}{4}\begin{pmatrix} 2(1+\gamma^2) & 0 & 1-\gamma^2 & \cdot & \cdot & \cdot & 1-\gamma^2 & 0 \\ 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & & 1-\gamma^2 \\ 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & \mathbf{0} & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ \cdot & & \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \mathbf{0} & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 \\ 1-\gamma^2 & & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 \\ 0 & 1-\gamma^2 & & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) \end{pmatrix}. \tag{2.16c}$$

The vectors are the real solutions of the eigenvalue equation

$$\phi_k(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \Lambda_k^2\phi_k\,. \tag{2.17}$$

A complete set of solutions is

$$\phi_{kj} = \begin{matrix} (2/N)^{\frac{1}{2}} \sin kj \\ (2/N)^{\frac{1}{2}} \cos kj \end{matrix} \tag{2.18a}$$

belonging to the set of eigenvalues

$$\Lambda_k^2 = 1 - (1 - \gamma^2)\sin^2 k, \tag{2.18b}$$

where

$$k = 2\pi m/N, \qquad m = -\tfrac{1}{2}N, \cdots, 0, 1, \cdots, \tfrac{1}{2}N - 1. \tag{2.18c}$$

In (2.18a) we take the upper solution for ϕ_{kj} if $k > 0$, the lower solution if $k \leqq 0$. For $\Lambda_k \neq 0$, $(A - 7a)$ gives

$$\psi_{kj} = \Lambda_k^{-1} (\cos k\, \phi_{kj} + \gamma \sin k\, \phi_{-kj}), \tag{2.18d}$$

while if $\Lambda_k = 0$

$$\psi_{kj} = \pm \phi_{kj}\,. \tag{2.18d'}$$

$\Lambda_k = 0$ is an eigenvalue only if $\gamma = 0$ and $N/4$ is an integer. To simplify the discussion, let us assume that $N/4$ is not an integer and therefore that $\Lambda_k \neq 0$.

The sign of Λ_k being arbitrary, we shall take it always to be positive. This corresponds to a particle-hole picture for the η-particles, where the ground state has no elementary fermions and the elementary fermion excitations both above and below the Fermi surface have positive energies.[2] Λ_k is shown in Fig. 1 for the isotropic and extreme anisotropic (Ising) cases and for one intermediate case. Remark that only for the isotropic case is there no energy gap.

The ground state Ψ_0 is the state with no elementary excitations:

$$\eta_k \Psi_0 = 0, \quad \text{all } k. \tag{2.19}$$

The ground-state energy, according to (A-12) is

$$E_0 = -\tfrac{1}{2} \sum_k \Lambda_k\,. \tag{2.20}$$

In the limit $N \to \infty$, the sum can be replaced by an integral giving

$$\begin{aligned} E_0/N &= -(\tfrac{1}{4}\pi) \int_{-\pi}^{\pi} dk\, [1 - (1 - \gamma^2) \sin^2 k]^{\frac{1}{2}} \\ &= -(1/\pi)\mathcal{E}(1 - \gamma^2), \end{aligned} \tag{2.21}$$

where $\mathcal{E}(k^2)$ is one of the complete elliptic integrals (*13*). E_0/N goes smoothly between the limiting cases

$$E_0/N = -1/\pi, \quad \text{isotropic case,} \quad \gamma = 0, \tag{2.22a}$$

and

$$E_0/N = -\tfrac{1}{2}, \quad \text{Ising case,} \quad \gamma = 1. \tag{2.22b}$$

[2] The "Fermi surface" consists of the points $k = \pm\pi/2$. The alternate picture in which all excitations are "particles" (in the isotropic case, a "particle" is an up spin) would be obtained by letting Λ_k have the sign of $\cos k$. The Fermi sea would then be defined by $|\, k\, | > \pi/2$. The particle-hole picture is preferred because it somewhat simplifies the algebra.

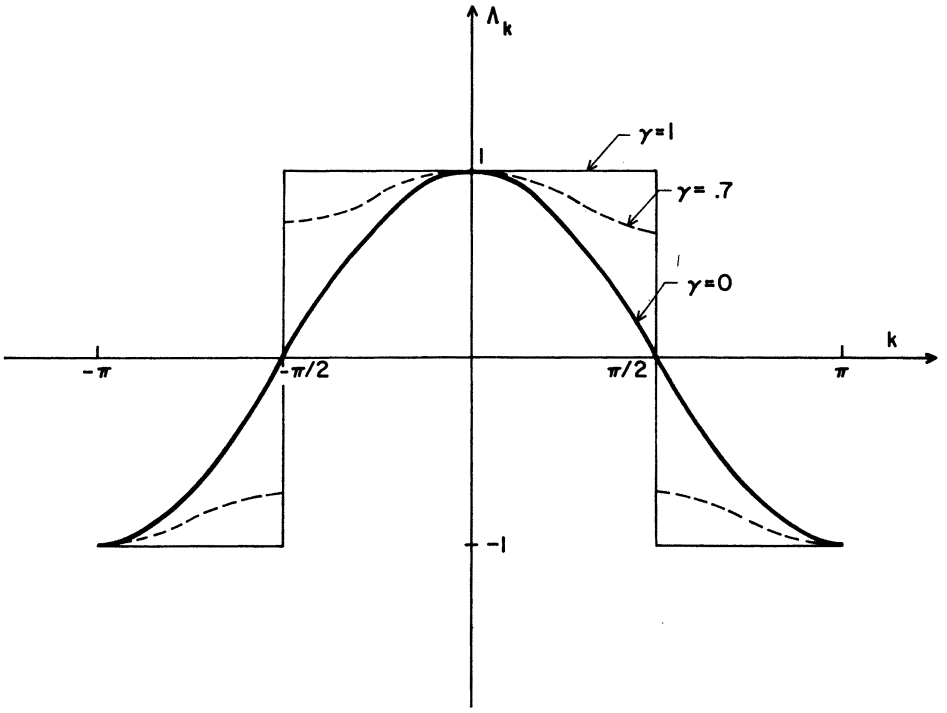

FIG. 1. Energy of elementary excitations in XY model as function of wave vector for three different degrees of anisotropy.

At this point let us remark on the simplification resulting from the consideration of the c-cyclic rather than the a-cyclic problem. According to (2.11′), the Hamiltonian for the a-cyclic problem is complicated by the presence of the term

$$-\tfrac{1}{2}[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}]\,(\exp(i\pi\mathfrak{N}) + 1).$$

Although $\mathfrak{N}$ is not invariant under the transformation (2.15), its evenness or oddness is invariant, so that $\exp(i\pi\mathfrak{N})$ is invariant. Now in the ground state of the c-cyclic problem, and in all states with an even number of excitations, the number of c-particles is odd (assuming $N/4$ is not an integer, the k's are occupied symmetrically around $k = 0$, except that $k = \pi$ but not $k = -\pi$ is occupied). Therefore, the additional term gives zero acting on such states and they remain eigenstates of the a-cyclic problem. States with an odd number of excitations, on the other hand, have $\mathfrak{N}$ even, giving the additional term

$$-\tfrac{1}{2}(c_N^\dagger c_1 + \gamma c_N^\dagger c_1 + \text{h.c.})$$

in the Hamiltonian. This has the effect of making changes of order $1/N$ in the

k's, ϕ_k's, and ψ_k's, all of which can be exactly calculated and are negligible in the calculation of real physical quantities. Strictly speaking though, the elementary excitations are not independent for the a-cyclic problem because of this dependence on the evenness or oddness of the total number of excitations present, and this is why we have preferred to consider the c-cyclic problem.

The free energy is the grand potential of such a system of noninteracting fermions with zero chemical potential ($\beta = 1/kT$):

$$F_\gamma/N = -kT\left[\ln 2 + \frac{2}{\pi}\int_0^{\pi/2} dk \ln\cosh\left(\tfrac{1}{2}\beta\Lambda_k\right)\right]. \tag{2.23}$$

In the isotropic limit we obtain

$$F_{\text{isotrop.}}/N = -kT\left[\ln 2 + \frac{2}{\pi}\int_0^{\pi/2} dk \ln\cosh\left(\tfrac{1}{2}\beta\cos k\right)\right]; \tag{2.24a}$$

while in the Ising limit, we obtain the classical result,

$$F_{\text{Ising}}/N = -kT(\ln 2 + \ln\cosh\tfrac{1}{2}\beta). \tag{2.24b}$$

Neither case exhibits any singular behavior as a function of temperature, a result to be expected in view of the one-dimensional nature of the model.

C. Short- and Long-Range Order in the Ground State

The long-range order for the Heisenberg model is often defined in terms of two sublattices (in the case of the linear chain, the sublattices of all even sites and of all odd sites). It is taken to be the preponderance of spins up to spins down on one of the sublattices, or of spins up on one sublattice to spins up on the other. Because of the invariance of the Hamiltonian under translations by any number of sites and also under 180° rotations about the x-, y-, and z-axes in spin space, it is clear that for a nondegenerate stationary state such a definition of long-range order must give zero, even if by any reasonable definition the state were ordered. That the ground state is nondegenerate is shown in Appendix B. The completely ferromagnetic states can have long-range order by this definition only because they are so highly degenerate. The definition has nevertheless been useful because the approximate states considered have not always had the full symmetry of the Hamiltonian. A much better measure of the long-range order is the quantity

$$\rho_{lm} = \langle\Psi_0 \mid \mathbf{S}_l\cdot\mathbf{S}_m \mid \Psi_0\rangle. \tag{2.25}$$

This is the contraction at $t = 0$, of the time-dependent spin correlation tensor

$$\varrho_{lm}(t) = \langle\Psi_0 \mid \mathbf{S}_l(0)\mathbf{S}_m(t) \mid \Psi_0\rangle \tag{2.26}$$

which enters in the calculation of any process, such as neutron scattering, con-

ceived to measure the order directly. Because of the nature of the model, we wish to calculate separately the various contributions to this order parameter:

$$\rho^x_{lm} = \langle\Psi_0 \mid S^x{}_l S^x{}_m \mid \Psi_0\rangle = \tfrac{1}{4}\langle\Psi_0 \mid (a_l^\dagger + a_l)(a_m^\dagger + a_m) \mid \Psi_0\rangle, \tag{2.27a}$$

$$\rho^y_{lm} = \langle\Psi_0 \mid S^y{}_l S^y{}_m \mid \Psi_0\rangle = \tfrac{1}{4}\langle\Psi_0 \mid (a_l^\dagger - a_l)(a_m^\dagger - a_m) \mid \Psi_0\rangle, \tag{2.27b}$$

$$\rho^z_{lm} = \langle\Psi_0 \mid S^z{}_l S^z{}_m \mid \Psi_0\rangle = \langle\Psi_0 \mid (a_l^\dagger a_l - \tfrac{1}{2})(a_m^\dagger a_m - \tfrac{1}{2}) \mid \Psi_0\rangle. \tag{2.27c}$$

We shall derive general expressions which reduce the calculation of these contributions to quadratures.

Consider ρ^x_{lm} in terms of the c's and $c^\dagger$'s:

$$\begin{aligned}\rho^x_{lm} &= \tfrac{1}{4}\left\langle \Psi_0 \middle| (c_l^\dagger + c_l) \exp\left(\pi i \sum_{l}^{m-1} c_i^\dagger c_i\right)(c_m^\dagger + c_m) \middle| \Psi_0 \right\rangle \\ &= \tfrac{1}{4}\left\langle \Psi_0 \middle| (c_l^\dagger - c_l) \exp\left(\pi i \sum_{l+1}^{m-1} c_i^\dagger c_i\right)(c_m^\dagger + c_m) \middle| \Psi_0 \right\rangle.\end{aligned} \tag{2.28}$$

Now observe that

$$\exp(\pi i c_i^\dagger c_i) = (c_i^\dagger + c_i)(c_i^\dagger - c_i), \tag{2.29a}$$

a result that is readily verified in the representation diagonalizing $c_i^\dagger c_i$. Defining

$$A_i = c_i^\dagger + c_i \quad \text{and} \quad B_i = c_i^\dagger - c_i, \tag{2.30}$$

we have

$$\rho^x_{lm} = \tfrac{1}{4}\langle\Psi_0 \mid B_l A_{l+1} B_{l+1} \cdots A_{m-1} B_{m-1} A_m \mid \Psi_0\rangle. \tag{2.31a}$$

In a similar way, using

$$\exp(\pi i c_i^\dagger c_i) = -(c_i^\dagger - c_i)(c_i^\dagger + c_i), \tag{2.29b}$$

we have

$$\rho^y_{lm} = (-1)^{m-l}\tfrac{1}{4}\langle\Psi_0 \mid A_l B_{l+1} A_{l+1} \cdots B_{m-1} A_{m-1} B_m \mid \Psi_0\rangle. \tag{2.31b}$$

Finally, because

$$a_i^\dagger a_i - \tfrac{1}{2} = -\tfrac{1}{2}(a_i^\dagger + a_i)(a_i^\dagger - a_i) = -\tfrac{1}{2}(c_i^\dagger + c_i)(c_i^\dagger - c_i), \tag{2.29c}$$

we have

$$\rho^z_{lm} = \tfrac{1}{4}\langle\Psi_0 \mid A_l B_l A_m B_m \mid \Psi_0\rangle. \tag{2.31c}$$

To evaluate expectation values such as appear in (2.31a, b, c), we make use of the well-known Wick Theorem[3] in quantum field theory, which allows us to express the vacuum expectation value of a product of operators, all of which

[3] See Wick (*14*) or subsequent books on quantum field theory.

obey anticommutation rules, in terms of so-called contractions of pairs, i.e., vacuum expectation values of products of just two operators. Explicitly, if $\mathcal{O}_1, \cdots, \mathcal{O}_{2n}$ are a set of such operators, then

$$\langle \Psi_0 \mid \mathcal{O}_1 \cdots \mathcal{O}_{2n} \mid \Psi_0 \rangle = \sum_{\text{all pairings}} (-1)^{p'} \prod_{\text{all pairs}} (\text{contraction of the pair}),$$

where the contraction $\langle \mathcal{O}_i \mathcal{O}_j \rangle$ is defined to be $\langle \Psi_0 \mid \mathcal{O}_i \mathcal{O}_j \mid \Psi_0 \rangle$, and where p' is the signature of the permutation, for a given pairing, necessary to bring operators of the same pair next to one another from the original order.

A particular simplification occurs in evaluating (2.31a, b, c) because certain kinds of contractions vanish. In fact, the basic contractions that arise are readily calculated:

$$\langle A_i A_j \rangle = \sum_k \phi_{ki} \phi_{kj} = \delta_{ij}, \tag{2.32a}$$

$$\langle B_i B_j \rangle = -\sum_k \psi_{ki} \psi_{kj} = -\delta_{ij}, \tag{2.32b}$$

$$\langle B_i A_j \rangle = -\langle A_j B_i \rangle = -\sum_k \psi_{ki} \phi_{kj} \equiv G_{ij}. \tag{2.32c}$$

Because $\langle A_i A_i \rangle$ and $\langle B_i B_i \rangle$ never occur, only pairings in which all contractions are of the type $\langle B_i A_j \rangle$ contribute in (2.31a, b, c).

The most straightforward pairing contributing to ρ^x_{lm} is

$$\langle B_l A_{l+1} \rangle \langle B_{l+1} A_{l+2} \rangle \cdots \langle B_{m-1} A_m \rangle.$$

All other pairings can be obtained from this one by permuting the A's among themselves with the B's fixed. Because the number of crossings of B's by A's is then always even, the sign associated with a given permutation is $(-1)^{p'}$, where p' is the signature of the permutation of the A's. Thus

$$\begin{aligned} \rho^x_{lm} &= \tfrac{1}{4} \sum_P (-1)^{p'} G_{l,P(l+1)} \cdots G_{m-1,P(m)} \\ &= \tfrac{1}{4} \begin{vmatrix} G_{l,l+1} & G_{l,l+2} & \cdots & G_{lm} \\ \vdots & & & \vdots \\ G_{m-1,l+1} & \cdots & & G_{m-1,m} \end{vmatrix}. \end{aligned} \tag{2.33a}$$

Similarly, because $A_l B_{l+1} = -B_{l+1} A_l$, etc.

$$\rho^y_{lm} = \tfrac{1}{4} \begin{vmatrix} G_{l+1,l} & G_{l+1,l+1} & \cdots & G_{l+1,m-1} \\ \vdots & & & \vdots \\ G_{ml} & \cdots & & G_{m,m-1} \end{vmatrix}. \tag{2.33b}$$

Thus, both ρ^x_{lm} and ρ^y_{lm} are particular subdeterminants of det $\mathbf{G}$. ρ^z_{lm} is immediately calculable from (2.31c) and Wick's theorem. For $l < m$,

$$\begin{aligned} \rho^z_{lm} &= \tfrac{1}{4}(\langle A_l B_l \rangle \langle A_m B_m \rangle - \langle A_l B_m \rangle \langle A_m B_l \rangle) \\ &= \tfrac{1}{4}(G_{ll} G_{mm} - G_{ml} G_{lm}). \end{aligned} \tag{2.33c}$$

Let us now consider the detailed properties of the G_{ij}'s. First observe that G_{ij}, considered as an element of an $N \times N$ matrix is just

$$G_{ij} = -(\psi^T \phi)_{ij}, \tag{2.34}$$

where ϕ and ψ are the matrices ϕ_{ki} and ψ_{ki}. It is immediately obvious that $\mathbf{G}$ is unitary because ϕ and ψ are unitary:

$$\mathbf{G}\mathbf{G}^T = \psi^T \phi \phi^T \psi = \psi^T \psi = \mathbf{1}. \tag{2.35}$$

The determinant of $\mathbf{G}$ is thus ± 1. The actual sign, which will be needed in the following section, is readily calculated:

$$\det \mathbf{G} = \det (-\psi^T \phi) = (-1)^N \det \psi^T \phi.$$

But from (A-7a)

$$(\psi^T)_{ik} = ((\mathbf{A} - \mathbf{B})^T \phi^T \mathbf{\Lambda}^{-1})_{ik},$$

where

$$(\mathbf{\Lambda})_{kk'} = \Lambda_k \delta_{kk'}.$$

Thus, using $\det \phi = \pm 1$, we obtain

$$\det \mathbf{G} = (-1)^N \det \mathbf{\Lambda}^{-1} \det (\mathbf{A} - \mathbf{B}).$$

Now $\det \mathbf{\Lambda}^{-1} > 0$, because $\Lambda_k > 0$ for all k. Thus

$$\det \mathbf{G} = (-1)^N \det (\mathbf{A} - \mathbf{B}) / | \det (\mathbf{A} - \mathbf{B}) |. \tag{2.36}$$

A second important property of G_{ij} is that, for the cyclic problem,

$$G_{ij} = G_{i-j} \equiv G_r, \tag{2.37}$$

a result which can be proved either from the invariance properties of the cyclic Hamiltonian or from direct evaluation of the sums in (2.32c).

To calculate G_r explicitly we consider the limit $N \to \infty$ with r fixed. It is shown in Appendix C that

$$G_r = -[\tfrac{1}{2}(1 + \gamma)L_{r+1} + \tfrac{1}{2}(1 - \gamma)L_{r-1}], \qquad r \text{ odd},$$

and

$$G_r = 0, \qquad r \text{ even}, \tag{2.38a}$$

where

$$L_r(\gamma) = (2/\pi) \int_0^{\pi/2} dk \cos kr \, [1 - (1 - \gamma^2) \sin^2 k]^{-\frac{1}{2}} = L_{-r}(\gamma). \tag{2.38b}$$

It is thus evident that $\gamma \to -\gamma$ is equivalent to $r \to -r$. In the isotropic limit

($\gamma = 0$), (2.38), reduces to

$$G_r = (-1)^{\frac{1}{2}(r+1)} 2/\pi r, \qquad r \text{ odd},$$

and

$$G_r = 0, \qquad r \text{ even}. \tag{2.39a}$$

In the extreme anisotropic limit ($\gamma = 1$)

$$G_{-1} = -1,$$

and

$$G_r = 0, \qquad r \neq -1. \tag{2.39b}$$

In the general anisotropic case, G_r is not so simply evaluated. The special cases of G_1 and G_{-1} (all that are needed for the nearest neighbor order in the cyclic chain) can be expressed in terms of the complete elliptic integrals (*13*) $\mathfrak{K}(k^2)$ and $\mathfrak{D}(k^2)$

$$G_{\pm 1} = -(2/\pi)[\mathfrak{K}(1-\gamma^2) - (1 \pm \gamma)\mathfrak{D}(1-\gamma^1)]. \tag{2.40}$$

The asymptotic behavior of G_r for $r \to \infty$, crucial for the long-range order, can be obtained by repeated integrations by parts. Assuming $\gamma \neq 0$ and r even, one finds for L_r

$$L_r(\gamma) = \frac{1}{r^4}[f^{(\mathrm{III})}(0) - (-1)^{\frac{1}{2}r} f^{(\mathrm{III})}(\pi/2)]$$

$$- \frac{1}{r^6}\left[f^{(\mathrm{IV})}(0) - (-1)^{\frac{1}{2}r} f^{(\mathrm{IV})}(\pi/2) + \int_0^{\pi/2} dk\, f^{(\mathrm{VI})}(k) \cos kr\right],$$

where

$$f(k) = (2/\pi)[1 - (1-\gamma^2)\sin^2 k]^{-\frac{1}{2}}. \tag{2.41}$$[4]

Thus for sufficiently large odd r

$$G_r \sim -\frac{1}{r^4}[f^{(\mathrm{III})}(0) + 2\gamma(-1)^{\frac{1}{2}(r-1)} f^{(\mathrm{III})}(\pi/2)] + O(1/r^6)$$

or

$$|G_r| < A/r^4 \quad \text{for} \quad |r| > r_0, \tag{2.42}$$

where A and r_0 are constants depending on γ but not on r. For general values of r, the following series for L_r (r even) is convenient:

$$L_r(\gamma) = (-1)^{\frac{1}{2}r} \frac{2}{1+\gamma}\left[g_0 g_{r/2} - \frac{1}{\pi}\ln(1-\lambda^2) - \sum_1^\infty \lambda^{2l}\left(\frac{1}{\pi l} - g_l g_{l+\frac{1}{2}r}\right)\right] \tag{2.43a}$$

[4] This behavior is found because $f'(0) = f'(\pi/2) = 0$, which is true only if $\gamma \neq 0$.

where

$$\lambda = (1 - \gamma)/(1 + \gamma) \tag{2.43b}$$

and

$$g_l = 2^{-2l}\binom{2l}{l} \underset{l\to\infty}{\sim} (\pi l)^{-\frac{1}{2}}. \tag{2.43c}$$

This series is readily obtained using the relations

$$[1 - (1 - \gamma^2)\sin^2 k]^{\frac{1}{2}} = [2/(1 + \gamma)] \sum_0^\infty (-\lambda)^m P_m(\cos 2k),$$

$$P_m(\cos 2k) = \sum_{l=0}^{m} g_l g_{m-l} \cos[(m - 2l)2k],$$

and

$$g_l \sim (\pi l)^{-\frac{1}{2}}.$$

Actual numerical evaluation for $\lambda^2 = \frac{2}{3}$ or $\gamma = 0.10102$ gives Table I. It should be remarked that L_r, G_r, the various contributions to the order parameter, and the ground-state energy are all nonanalytic functions of γ at the point $\gamma = 0$, although they are analytic at $\gamma = \pm 1$. This is, of course, the reason for the different asymptotic behavior of G_r for $\gamma = 0$ and $\gamma \neq 0$. This suggests that a perturbation treatment should converge if the totally anisotropic case is considered as the zeroth order Hamiltonian, a result observed by Walker (*9*) for the full anisotropic Heisenberg model of the antiferromagnetic chain.

We now investigate the short-, intermediate-, and long-range order for the

TABLE I

QUANTITIES USEFUL IN CALCULATING ORDER BETWEEN DIFFERENT SPINS FOR THE XY MODEL WITH $\gamma = 0.10102$

r	$\frac{1}{2}(1+\gamma)L_{r-1}$	G_r	G_{-r}
1	1.2917	−0.4560	−0.8029
3	−0.5986	0.1047	0.2850
5	0.3841	−0.0455	−0.1652
7	−0.2680	0.0242	0.1091
9	0.1946	−0.0143	−0.0765
11	−0.1446	0.0089	0.0555
13	0.1092	−0.0058	−0.0412
15	−0.0833	0.0039	0.0310
17	0.0641	−0.0027	−0.0236
19	−0.0497		

cyclic case. The various contributions to the short-range order are readily calculated:

$$\rho_{i,i+1}^{x} \equiv \rho_1^{x} = \tfrac{1}{4}G_{-1}$$
$$= -(2\pi)^{-1}[\mathfrak{K}(1-\gamma^2) - (1-\gamma)\mathfrak{D}(1-\gamma^2)], \tag{2.44a}$$

$$\rho_{i,i+1}^{y} \equiv \rho_1^{y} = \tfrac{1}{4}G_1$$
$$= -(2\pi)^{-1}[\mathfrak{K}(1-\gamma^2) - (1+\gamma)\mathfrak{D}(1-\gamma^2)], \tag{2.44b}$$

$$\rho_{i,i+1}^{z} \equiv \rho_1^{z} = -\tfrac{1}{4}G_1G_{-1}$$
$$= -\pi^{-2}[(\mathfrak{K}(1-\gamma^2) - \mathfrak{D}(1-\gamma^2))^2 - \gamma^2(\mathfrak{D}(1-\gamma^2))^2]. \tag{2.44c}$$

We plot these parameters and the total order $\rho_1 \equiv \rho_1^{x} + \rho_1^{y} + \rho_1^{z}$ as functions of γ in Fig. 2.

For the intermediate-range order one must fall back on a numerical evalua-

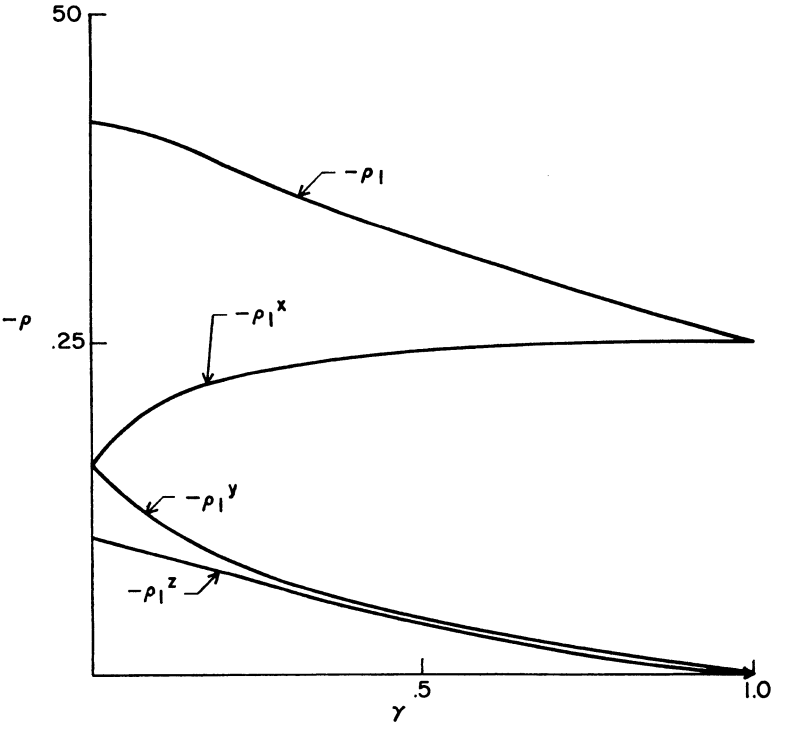

FIG. 2. Various contributions to the short-range order as functions of the degree of anisotropy in the XY model.

tion of the relevant determinants. Because $G_r = 0$ for even r, these determinants simplify somewhat. Thus

$$\rho^x_{2n-1} = \tfrac{1}{4}R_{n-1}R_n \tag{2.45a}$$

and

$$\rho^x_{2n} = \tfrac{1}{4}R_n^2 \tag{2.45b}$$

where

$$R_n = \begin{vmatrix} G_{-1} & G_{-3} & \cdots & & G_{-(2n-1)} \\ G_1 & G_{-1} & G_{-3} & & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & & \cdot & \cdot\ \cdot & \\ & & & G_1\ G_{-1} & G_{-3} \\ G_{2n-3} & & & G_1 & G_{-1} \end{vmatrix} \tag{2.46a}$$

and

$$R_0 = 1. \tag{2.46b}$$

Similar expressions can be derived for ρ^y_{2n-1} and ρ^z_{2n}. One has only to let $G_r \to G_{-r}$. Numerical evaluation of this determinant for several values of n leads to a very slowly converging sequence for ρ_n, even for $\gamma = 0$, the case expected to be most rapidly converging. Results for $\gamma = 0$ and $\gamma = 0.10102$ are summarized as shown in the tabulation.

n	1	2	3	4	5	6
$\rho_n(\gamma = 0)$	−0.1592	0.1013	−0.0860	0.0730	−0.0661	0.0597
$\rho_n(\gamma = 0.10102)$	−0.2007	0.1611	−0.1555	0.1500	−0.1483	0.1467

Now let us investigate the long-range order. The cases $\gamma = 0$ and $\gamma \neq 0$ exhibit entirely different long-range order characteristics because of the difference in asymptotic behavior of G_r for these two cases. We first consider the isotropic case, which is simpler and, as we now show, has no long-range order.

We seek the limits of ρ_n^x, ρ_n^y, and ρ_n^z as $n \to \infty$ for $\gamma = 0$. The fact that we have first taken the limit $N \to \infty$ in passing from sums to integrals ensures that we never come round the circle when $n \to \infty$.

$$\rho_n{}^x = \rho_n{}^y = \frac{1}{4}\begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-n} \\ G_0 & G_{-1} & G_{-2} & \\ \cdot & & \cdot & \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \\ & & \cdot & G_{-2} \\ G_{n-2} & & G_0 & G_{-1} \end{vmatrix} \equiv \frac{1}{4} D_n , \tag{2.47a}$$

$$\rho_n{}^z = \tfrac{1}{2}\delta_{n0} - \tfrac{1}{4} G_n G_{-n} \xrightarrow[n \to \infty]{} -(\pi n)^{-2} \to 0. \tag{2.47b}$$

An upper bound to $| D_n |$ may be obtained with Hadamard's Theorem (*15*), which states that

$$| \det_n \mathbf{C} |^2 \leqq \prod_{i=1}^{n} \left(\sum_{j=1}^{n} C_{ij}^2 \right) \equiv \prod_{i=1}^{n} d_{i,n}^2 , \tag{2.48}$$

if $d_{i,n}$ is the norm of the ith row of $\mathbf{C}$. The equality holds only when the rows are all mutually orthogonal. We divide the rows of D_n into three groups, those near the top (the first n_0 rows, where n_0 is independent of n and $\ll n$), those near the bottom (the last n_0 rows) and those in the middle. Because $d_{i,n}^2 \leqq 1$ for all i from the unitarity of $\mathbf{G}$, we may replace $d_{i,n}$ by 1 for the first and third groups in (2.48):

$$D_n{}^2 \leqq \prod_{i=n_0+1}^{n-n_0} d_{i,n}^2 . \tag{2.49}$$

In the middle group

$$\begin{aligned} d_{i,n}^2 = \sum_{j=1}^{n} G_{i-1-j}^2 &= 1 - 2 \sum_{M(i,n)}^{\infty} G_r^2 - \sum_{m(i,n)}^{M(i,n)-1} \\ G_r{}^2 &\leqq \exp\left[-2 \sum_{M}^{\infty} G_r{}^2 - \sum_{m}^{M-1} G_r{}^2 \right], \end{aligned} \tag{2.50}$$

where

$$M(i,n) = \max\,(i - 1, n + 2 - i) \tag{2.51a}$$

and

$$m(i,n) = \min\,(i - 1, n + 2 - i). \tag{2.51b}$$

But

$$\sum_{0}^{b} G_r{}^2 \geqq (2/\pi)^2 \frac{1}{2} \int_{a+1}^{b} k^{-2}\, dk = (2/\pi)^2 \frac{1}{2} \left(\frac{1}{a+1} - \frac{1}{b} \right), \tag{2.52}$$

so that

$$\prod_{i=n_0+1}^{n-n_0} d_{i,n}^2 \leqq \exp\left\{-(2/\pi)^2 \frac{1}{2}\left[\sum_{n_0+1\leqq i\leqq \frac{1}{2}(n+3)} \left(\frac{1}{n+2-i}+\frac{1}{i}\right) + \sum_{\frac{1}{2}(n+3)<i\leqq n-n_0} \left(\frac{1}{i-1}+\frac{1}{n+3-i}\right)\right]\right\}. \tag{2.53}$$

Furthermore

$$\sum_a^b (1/k) \geqq \int_a^b (dk/k) = \ln(b/a),$$

so that each sum in the exponent of (2.53) can be replaced by a lower bound:

$$D_n^2 \leqq \exp\left\{-(2/\pi)^2 \frac{1}{2}\left[\ln 2\left(\frac{n-n_0+1}{n+1}\right) + \ln 2\left(\frac{n-n_0-1}{n+1}\right) + \ln \frac{1}{2}\left(\frac{n+3}{n_0+1}\right) + \ln \frac{1}{2}\left(\frac{n+3}{n_0+3}\right)\right]\right\}. \tag{2.54}$$

As $n \to \infty$

$$D_n^2 \leqq (n+3)^{-(2/\pi)^2} \times \text{constant}, \tag{2.55}$$

and so

$$\rho_n^x = \rho_n^y \to 0 \quad \text{as} \quad n \to \infty. \tag{2.56}$$

When $\gamma \neq 0$, $|G_r| < Ar^{-4}$ for $r > r_0$ and the preceding development gives only the very weak result

$$D_n^2 \leqq \text{constant} \quad \text{as} \quad n \to \infty,$$

which does not exclude the possibility that either ρ_n^x, ρ_n^y, or both approach finite limits as $n \to \infty$ (n even). Not only the norms of the rows but the overlap between rows must now be considered to improve the estimate. Conceivably a more powerful theorem would show that either or both the order parameters tend to zero as $n \to \infty$, although no such theorem has been found. Instead, when we consider the spins at the ends of a long chain with free ends, we find for $\gamma > 0$ that $\rho_{iN}^x \neq 0$ although $\rho_{iN}^y = O(1/N)$ (and the reverse for $\gamma < 0$), as we now show.

D. End-to-End Order in the Ground State

It is easy to calculate the order between the first and last spins of a chain of N spins, even if evaluation of the intermediate-range order is difficult. This is

because what is involved is an $(N-1)\times(N-1)$ minor of the $N\times N$ determinant det **G**, where **G** is unitary. Thus

$$\rho^x_{iN} = \tfrac{1}{4}\begin{vmatrix} G_{12} & \cdots & G_{1N} \\ \vdots & & \vdots \\ G_{N-1,2} & \cdots & G_{N-1,N} \end{vmatrix} = (-1)^{N-1}\tfrac{1}{4}(\mathbf{G}^{-1})_{1N}\det \mathbf{G}. \quad (2.57)$$

Because **G** is unitary

$$(\mathbf{G}^{-1})_{1N} = G_{N1}\,. \quad (2.58)$$

Therefore, using (2.36), we have

$$\rho^x_{1N} = (-1)^{N-1}\,\tfrac{1}{4}G_{N1}\det \mathbf{G} = -\tfrac{1}{4}G_{N1}\det(\mathbf{A}-\mathbf{B})/|\det(\mathbf{A}-\mathbf{B})|. \quad (2.59a)$$

We have assumed only that $\Lambda_k \neq 0$ for all k. In a similar way

$$\rho^y_{1N} = -\tfrac{1}{4}G_{1N}\det(\mathbf{A}-\mathbf{B})/|\det(\mathbf{A}-\mathbf{B})|. \quad (2.59b)$$

As before

$$\rho^z_{1N} = \tfrac{1}{4}\,(G_{11}G_{NN} - G_{1N}G_{N1}). \quad (2.59c)$$

An alternative way to derive (2.59a,b) which bypasses the general problem of calculating ρ_{lm}, is as follows:

$$\rho^x_{1N} = \tfrac{1}{4}\,\langle\Psi_0\,|\,(c_1^\dagger + c_1)(c_N^\dagger - c_N)\exp\,(i\pi\mathfrak{N})\,|\,\Psi_0\rangle. \quad (2.60)$$

Because $[\exp\,(i\pi\mathfrak{N}),\, H_\gamma] = 0$, the nondegeneracy of Ψ_0 (assured by $\Lambda_k \neq 0$) implies that Ψ_0 is an eigenstate of $\exp(\pi i\mathfrak{N})$ belonging to one of the eigenvalues ± 1. Thus $\rho^x_{1N} = \mp\,\tfrac{1}{4}G_{N1}$. To determine which sign is in fact correct, we use the fact that the sign is independent of the continuous variable γ, and evaluate it for $\gamma = 0$. We find finally

$$\rho^x_{1N} = -\tfrac{1}{4}G_{N1}\det \mathbf{A}/\,|\det \mathbf{A}\,|\,, \quad (2.61)$$

which agrees with (2.59a) providing $\Lambda_k \neq 0$ for all k (and thus $\det(\mathbf{A}-\mathbf{B}) \neq 0$ and $\det \mathbf{A} \neq 0$). For the cyclic chain the simplicity of the end-to-end order is of no interest because the sites 1 and N are nearest neighbors, and we obtain only the short-range order. For the chain with free ends, however, this is indeed a measure of the long-range order as $N \to \infty$. Certainly, if there is a finite end-to-end order, then there is finite long-range order as defined in the previous section, although the two calculations may give slightly different numerical results because of end effects. We investigate these end effects at the end of this section.

Consider then a chain of N spins with free ends. To ensure that Ψ_0 be non-

degenerate, or equivalently that $\Lambda_k \neq 0$ for all k, we assume N to be even.[5] We are then calculating the order between two spins that have a tendency, however small, to be antiparallel.

The relevant matrices are

$$\mathbf{A}-\mathbf{B}=\tfrac{1}{2}\begin{pmatrix} 0 & 1-\gamma & & & & & & \\ 1+\gamma & 0 & 1-\gamma & & & & \mathbf{0} & \\ & \ddots & \ddots & \ddots & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & 1+\gamma & 0 & 1-\gamma & \\ & \mathbf{0} & & & & 1+\gamma & 0 & \end{pmatrix} = (\mathbf{A}+\mathbf{B})^T, \quad (2.62)$$

$$(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$$

$$=\tfrac{1}{4}\begin{pmatrix} (1-\gamma)^2 & 0 & 1-\gamma^2 & & & & & \\ 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & \mathbf{0} & \\ 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \\ & \mathbf{0} & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 \\ & & & & & 1-\gamma^2 & 0 & (1+\gamma)^2 \end{pmatrix}. \quad (2.63)$$

Because the problem is no longer cyclic, the first, second, $(N-1)$st and Nth rows of $(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$ are different from all the rest.

The vectors ϕ_k and ψ_k are readily found and are of two kinds.

Modes of the first kind:

[5] It is readily seen that for N odd, $\det(\mathbf{A}-\mathbf{B})=0$, so there exists a zero eigenvalue of $(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$. The existence of this excitation corresponds to the fact that because both $R_x \equiv \exp[\pi i \sum_1^N S^x{}_i]$ and $R_z \equiv \exp[\pi i \sum_1^N S^z{}_i]$ commute with H and because there are an odd number of sites, every eigenstate is degenerate. Suppose Ψ is an eigenstate of H and R_z so that $R_z\Psi = \pm i\Psi$ (the eigenvalues of R_z are $\pm i$ for an odd number of spins). Then $\Psi' \equiv R_x\Psi$ is distinct from Ψ because $R_z\Psi' = \mp i\Psi'$ and yet it is an energy eigenstate degenerate with Ψ.

$$\phi_k^{\mathrm{I}} = A_k \begin{pmatrix} 0 \\ \sin 2k \\ 0 \\ \sin 4k \\ \vdots \\ 0 \\ \sin Nk \end{pmatrix} \quad \text{and} \quad \psi_k^{\mathrm{I}} = -A_k \delta_k \begin{pmatrix} \sin Nk \\ 0 \\ \sin(N-2)k \\ 0 \\ \vdots \\ \sin 2k \\ 0 \end{pmatrix}, \tag{2.64a}$$

where

$$\delta_k = \text{sign of } \cos(N+1)k, \tag{2.64b}$$

$$\Lambda_k = [1 - (1-\gamma^2)\sin^2 k]^{\frac{1}{2}}, \tag{2.64c}$$

and A_k is the normalization constant,

$$A_k \equiv \left[\sum_{n=1}^{N/2} \sin^2 2nk\right]^{-\frac{1}{2}} = 2\left[N + 1 - \frac{\sin 2(N+1)k}{\sin 2k}\right]^{-\frac{1}{2}}. \tag{2.64d}$$

The k's are the roots of the equation

$$\sin(N+2)k/\sin Nk = (1-\gamma)/(1+\gamma) = -\lambda, \tag{2.64e}$$

which we discuss below. It can then be shown that

$$\Lambda_k = \cos k / \,|\cos(N+1)k\,|\,. \tag{2.64f}$$

The parameter λ, previously introduced in (2.43b), is a convenient alternate characterization of the anisotropy, the isotropic case corresponding to $\lambda = 1$ and the Ising limits being $\lambda = 0, \infty$.

Modes of the second kind:

$$\phi_k^{\mathrm{II}} = A_k \begin{pmatrix} \sin Nk \\ 0 \\ \sin(N-2)k \\ 0 \\ \vdots \\ \sin 2k \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_k^{\mathrm{II}} = -A_k \delta_k \begin{pmatrix} 0 \\ \sin 2k \\ 0 \\ \sin 4k \\ \vdots \\ 0 \\ \sin Nk \end{pmatrix}, \tag{2.65a}$$

where δ_k, Λ_k, and A_k are as before, and the k's are the roots of the equation

$$\sin(N+2)k/\sin Nk = -1/\lambda. \tag{2.65b}$$

Assuming $\gamma > 0$, we represent the functions $\sin(N+2)k/\sin Nk$, λ, and $1/\lambda$ diagrammatically in Fig. 3. The roots of (2.64e) are of the form

$$k_m^{\mathrm{I}} = (\pi/N)(m - \nu_m^{\mathrm{I}}) + O(1/N^2), \qquad m = 1, \cdots, \tfrac{1}{2}N, \tag{2.66}$$

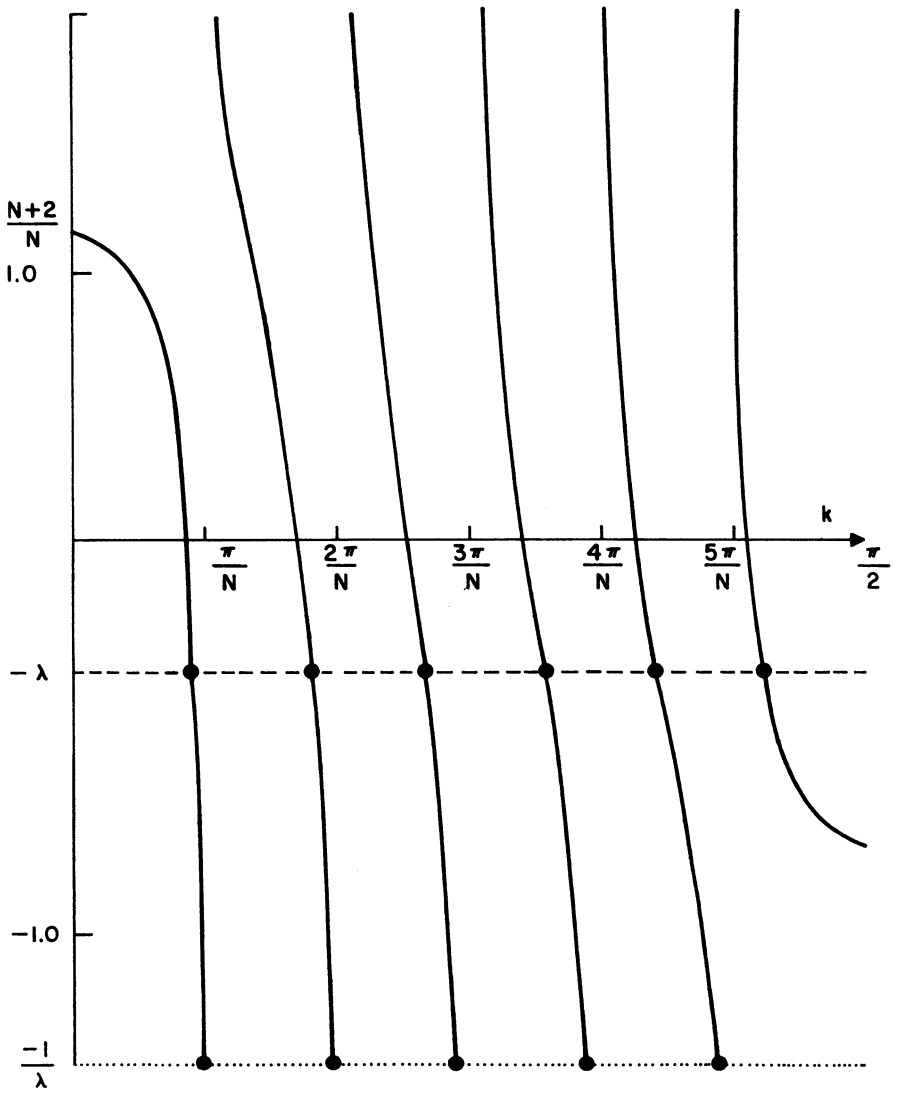

FIG. 3. Sin $(N+2)k/\sin Nk$ (continuous curve), $-\lambda$ (dashed line) and $-1/\lambda$ (dotted line) versus k for $N = 12$ and a typical value of λ. The intersections of these curves define the k^{I}'s and k^{II}'s in the XY model with free ends.

where $\nu_m{}^{\mathrm{I}}$, defined by

$$\cot \nu_m{}^{\mathrm{I}}\pi = [\lambda + \cos(2m\pi/N)]/\sin(2m\pi/N), \tag{2.67}$$

is found to be

$$\nu_m{}^{\mathrm{I}} = (m/N) + (1/\pi) \tan^{-1} [\gamma \tan(m\pi/N)]. \tag{2.67'}$$

Similarly, the *real* roots of (2.65b) are of the form

$$k_m^{\mathrm{II}} = (\pi/N)(m - \nu_m^{\mathrm{II}}) + O(1/N^2), \qquad m = 1, \cdots, \tfrac{1}{2}N - 1, \quad (2.68)$$

where

$$\nu_m^{\mathrm{II}} = (m/N) - (1/\pi)\tan^{-1}[\gamma \tan(m\pi/N)]. \quad (2.69)$$

There is also one complex root of (2.65b) which is very important:

$$k_0 = (\pi/2) + iv, \quad (2.70)$$

where v is the solution of

$$\cosh 2v + \coth Nv \sinh 2v = 1/\lambda. \quad (2.71)$$

In the zeroth approximation, we may set $\coth NV = 1$, so that

$$e^{2v} = 1/\lambda = (1 + \gamma)/(1 - \gamma). \quad (2.72)$$

In the next approximation

$$e^{2v} = 1/\lambda - (1 - \lambda^2)\lambda^{N-1} = \left(\frac{1+\gamma}{1-\gamma}\right) - \frac{4\gamma}{(1+\gamma)^2}\left(\frac{1-\gamma}{1+\gamma}\right)^{N-1}. \quad (2.72')$$

The ϕ and ψ vectors for this special mode are

$$\phi_{k_0} = A_{k_0}\begin{pmatrix} \sinh Nv \\ 0 \\ \vdots \\ (-1)^{\frac{1}{2}N-2}\sinh 4v \\ 0 \\ (-1)^{\frac{1}{2}N-1}\sinh 2v \\ 0 \end{pmatrix}$$

$$\text{and } \psi_{k_0} = (-1)^{\frac{1}{2}N+1}\begin{pmatrix} 0 \\ (-1)^{\frac{1}{2}N-1}\sinh 2v \\ 0 \\ (-1)^{\frac{1}{2}N-2}\sinh 4v \\ 0 \\ \vdots \\ 0 \\ \sinh Nv \end{pmatrix}, \quad (2.73a)$$

where

$$A_{k_0}^2 = 4\left[\frac{\sinh 2(N+1)v}{\sinh 2v} - N - 1\right]^{-1}$$
$$\simeq 4(1 - \lambda^2)\lambda^N = 16(\gamma/(1+\gamma)^2)\left(\frac{1-\gamma}{1+\gamma}\right)^N. \quad (2.73b)$$

This exhausts the normal modes because, for any mode with k' in $(\frac{1}{2}\pi, \pi)$, there is a mode with $k = \pi - k'$ that differs from the first only by a sign.

It is obvious from (2.64c) that $\Lambda_k > 0$ for all real k's. It is also readily seen that for the special mode k_0

$$\Lambda_{k_0} \simeq (1 + \lambda)\lambda^{N/2} = [2/(1 + \gamma)]\,[(1 - \gamma)/(1 + \gamma)]^{\frac{1}{2}N}. \tag{2.73c}$$

Thus, although the ground state is, strictly speaking, nondegenerate for any finite N, it becomes degenerate with the state carrying the k_0 excitation in the limit $N \to \infty$. It is observed in the next section that these two states have the same end-to-end order to $O(1/N)$. In terms of the customary definition of long-range order, the preponderance of spins up on one sublattice to spins up on the other, neither of these states shows any long-range order, if by "spins up" we mean spins in the x-direction. However, a linear combination of these two states in equal proportions will show a long-range order according to the customary definition.

We can now compute the various relevant G functions, recalling that $G_{ij} = -\sum_k \psi_{ki}\phi_{kj}$:

$$G_{1N} = \sum_{k^{\mathrm{I}}} A_k^{\,2}\,\delta_k \sin^2 Nk, \tag{2.74a}$$

$$G_{N1} = \sum_{k^{\mathrm{II}}\ \mathrm{real}} A_k^{\,2}\,\delta_k \sin^2 Nk + A_{k_0}^2\,(-1)^{\frac{1}{2}N} \sinh^2 Nv. \tag{2.74b}$$

Except for the factor δ_k, the summands in (2.74) are slowly varying functions of k, as shown in Appendix D, and each term is $O(1/N)$. The factor δ_k alternates in sign, the first δ_k being -1, etc. Thus a pair of consecutive terms in the summand is approximately

$$(d/dm)\,(A_{k_m}^2 \sin^2 Nk_m)$$

and the sums go over to Riemann integrals:

$$\tfrac{1}{2}\int_0^{\frac{1}{2}N} (d/dm)(A_{k_m}^2 \sin^2 Nk_m)\,dm = O(1/N). \tag{2.75}$$

Finally we have

$$G_{1N} = O(1/N), \tag{2.76a}$$

$$\begin{aligned} G_{N1} &= A_{k_0}^2\,(-1)^{\frac{1}{2}N} \sinh^2 Nv + O(1/N) \\ &= (-1)^{\frac{1}{2}N}\,(1 - \lambda^2) + O(1/N). \end{aligned} \tag{2.76b}$$

To calculate the end-to-end order in the ground state using (2.59), we note that

$$\det(\mathbf{A} - \mathbf{B}) = (-1)^{\frac{1}{2}N}\,(1 - \gamma^2)^{\frac{1}{2}N} \tag{2.77}$$

so that

$$\rho^x_{1N} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G_{N1} \tag{2.78a}$$

and

$$\rho^y_{1N} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G_{1N} . \tag{2.78b}$$

Because $G_{1N} = O(1/N)$, only ρ^x_{1N} of the order parameters is finite for $\gamma > 0$ as $N \to \infty$.

$$\rho^x_{1N} = -\tfrac{1}{4}(1 - \lambda^2) + O(1/N) = -[\gamma/(1 + \gamma)^2] + O(1/N). \tag{2.79}$$

The ground state of the one-dimensional XY model thus shows no end-to-end order in the isotropic case, but a finite end-to-end order for any finite amount of anisotropy.

As anticipated, we see explicitly that the various contributions to the order parameter are nonanalytic functions of γ at $\gamma = 0$. The limiting contribution $\rho^x_{1\infty}$, for example, is finite for $\gamma > 0$ but zero for $\gamma < 0$.

As we have already remarked, the order ρ^x_{1N} may differ from $\lim_{n\to\infty} \rho_n{}^x$ obtained for the cyclic chain because of end effects. To see how important these effects are, it is useful to compute the order between two spins situated near but not at the two ends of the chain. Somewhat simpler is the "end-to-almost-end" order calculated between the qth spin and the Nth spin, where q is small. Just as ρ^x_{1N} can be expressed with a 1×1 determinant, ρ^x_{qN} can be expressed with a $q \times q$ determinant as we now show.

$$\begin{aligned}
\rho^x_{qN} &= \tfrac{1}{4} \langle \Psi_0 \mid (a_q{}^\dagger + a_q)(a_N{}^\dagger + a_N) \mid \Psi_0 \rangle, \\
&= \tfrac{1}{4} \left\langle \Psi_0 \middle| \exp\left(i\pi \sum_1^{q-1} c_j{}^\dagger c_j \right)(c_q{}^\dagger + c_q)(c_N{}^\dagger + c_N) \exp\left(i\pi \sum_1^{N-1} c_j{}^\dagger c_j \right) \middle| \Psi_0 \right\rangle, \\
&= \tfrac{1}{4} \langle \Psi_0 \mid A_1 B_1 A_2 B_2 \cdots A_{q-1} B_{q-1} A_q B_N e^{i\pi\mathfrak{N}} \mid \Psi_0 \rangle.
\end{aligned} \tag{2.80}$$

But according to (2.61),

$$\exp(i\pi\mathfrak{N}) \mid \Psi_0 \rangle = (\det \mathbf{A} / \mid \det \mathbf{A} \mid) \mid \Psi_0 \rangle = (-1)^{\frac{1}{2}N} \mid \Psi_0 \rangle. \tag{2.81}$$

The evaluation of ρ^x_{qN} now gives, using Wick's theorem,

$$\rho^x_{qN} = \frac{(-1)^q(-1)^{\frac{1}{2}N}}{4} \begin{vmatrix} G_{11} & G_{12} & \cdots & G_{1q} \\ G_{21} & G_{22} & \cdots & G_{2q} \\ \vdots & \vdots & & \vdots \\ G_{q-1,1} & G_{q-1,2} & & G_{q-1,q} \\ G_{N1} & G_{N2} & & G_{Nq} \end{vmatrix} . \tag{2.82}$$

ρ^y_{qN} is obtained by letting $G_{ij} \to G_{ji}$. It should be borne in mind that the G_{ij}'s are now calculated for the chain with free ends; they are not the G_{ij}'s discussed

in the last section. We introduce the notation G^f_{ij} and G^c_{ij} for the free chain and cyclic chain, respectively. Then there are simple relations, proved in Appendix E, between the two kinds of G's provided $|i-j| = o(N)$.

$$G^f_{ij} = G^c_{i-j} - G^c_{i+j} \qquad \text{for } i \text{ odd}, j \text{ even}; \tag{2.83a}$$

$$G^f_{ij} = G^c_{i-j} - G^c_{-(i+j)} \qquad \text{for } i \text{ even}, j \text{ odd}; \tag{2.83b}$$

$$G^f_{ij} = 0 \qquad \text{for } i-j \text{ even}. \tag{2.83c}$$

The determinant in (2.82) can be simplified in two ways. First recall that

$$\rho^x_{1N} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G^f_{N1} \tag{2.78a}$$

and observe that if j is odd and $j = o(N)$,

$$G^f_{Nj} = (-1)^{\frac{1}{2}(j-1)} \lambda^{j-1}, \tag{2.84}$$

so that (2.82) simplifies to

$$\rho^x_{qN} = (-1)^{q-1} \rho^x_{1N} \begin{vmatrix} G^f_{11} & \cdots & G^f_{1q} \\ \vdots & & \\ G^f_{q-1,1} & \cdots & G^f_{q-1,q} \\ 1 \;\; 0 & -\lambda^2 \;\; 0 \;\; \lambda^4 & \cdots \end{vmatrix}. \tag{2.85}$$

Second, because of (2.83), the determinant can be simplified in analogy with (2.45a, b) giving

$$\rho^x_{2q,N} = (-1)^{q+1} S_q T_q \rho^x_{1N}, \tag{2.86a}$$

$$\rho^x_{2q-1,N} = (-1)^{q+1} S_q T_{q-1} \rho^x_{1N}, \tag{2.86b}$$

where

$$T_q = \begin{vmatrix} G^f_{12} & G^f_{14} & \cdots & G^f_{1,2q} \\ G^f_{32} & G^f_{34} & \cdots & G^f_{3,2q} \\ \vdots & \vdots & & \vdots \\ G^f_{2q-1,2} & G^f_{2q-1,4} & \cdots & G^f_{2q-1,2q} \end{vmatrix} \tag{2.87a}$$

and

$$S_q = \begin{vmatrix} G^f_{21} & G^f_{23} & \cdots & G^f_{2,2q-1} \\ G^f_{41} & G^f_{43} & \cdots & G^f_{4,2q-1} \\ \vdots & & & \vdots \\ G^f_{2q-2,1} & & \cdots & G^f_{2q-2,2q-1} \\ 1 & (i\lambda)^2 & \cdots & (i\lambda)^{2q-2} \end{vmatrix}. \tag{2.87b}$$

Numerical evaluation of ρ^x_{qN}/ρ^x_{1N} for $\gamma = 0.10102$ and $q = 2, 3, \cdots, 7$ shows a rapid convergence to a value differing by only a few percent from unity; but surprisingly, the order does not increase in absolute value monotonically as q increases.

E. Order in Excited States and at Finite Temperatures

The order parameters in excited states are given by simple modifications of (2.33). For example, the state with the elementary excitations $k_1, \cdots, k_s$ excited can be regarded as the vacuum state of a new set of η_k operators, where η_k and $\eta_k^\dagger$ are interchanged for $k_1, \cdots, k_s$. For these k's, this is equivalent to letting $\psi_{ki} \to -\psi_{ki}$ and $\Lambda_k \to -\Lambda_k$. Instead of (2.32c) we have

$$G_{ij}(k_1 \cdots k_s) = -\sum_{k \text{ unexc.}} \psi_{ki}\phi_{kj} + \sum_{k \text{ exc.}} \psi_{ki}\phi_{kj}. \tag{2.88}$$

Because s of the Λ_k's now are negative,

$$\det \mathbf{G}(k_1 \cdots k_s) = (-1)^s \det \mathbf{G}. \tag{2.89}$$

For the cyclic chain, the change of sign of a few of the terms contributing to G_{ij}, as given in (2.88) has a negligible effect on G_{ij}, because each term is $O(1/N)$. Thus in very low-lying excited states, the order between spins a fixed distance apart, (as $N \to \infty$) is the same as in the ground state, although this in itself does not imply long-range order at finite temperatures. For the end-to-end order in the chain with free ends, the sign of the order is changed with each additional excitation (except for k_0) because det **G** changes sign, so that at finite temperatures the end-to-end order vanishes. It is interesting to note, however, that for the one extremely low-lying excitation k_0, *both* det **G** *and* G_{N1} change sign so that this very low-lying excited state has the same end-to-end order as the ground state, to order $O(1/N)$.

The systematic generalization to finite temperatures of the treatment of order using Wick's theorem is simply achieved by introducing temperature-dependent contractions (*16*):

$$\langle B_i A_j \rangle = \operatorname{tr}[B_i A_j \exp(-\beta H_\gamma)]/\operatorname{tr} \exp(-\beta H_\gamma) \equiv G_{ij}(\beta). \tag{2.90}$$

The explicit evaluation of G_{ij} at finite temperatures is given in Appendix C. In matrix notation

$$\mathbf{G}(\beta) = -\boldsymbol{\psi}^T \tanh(\tfrac{1}{2}\beta\boldsymbol{\Lambda})\boldsymbol{\phi}. \tag{2.91}$$

$G(\beta)$ is no longer a unitary matrix. In fact, the norm of the entire ith row is

$$d_{i,N}(\beta) = \left[\sum_{j=1}^{N} (G_{ij}(\beta))^2\right]^{\frac{1}{2}} \leqq \tanh(\tfrac{1}{2}\beta\Lambda_{\max}) < 1. \tag{2.92}$$

Thus, even though $G_{i-j}(\beta) \sim A(\beta)/(i-j)^4$ for *all*[6] γ, the long-range order is zero at any finite temperature by Hadamard's theorem. In fact

$$\rho_n^x \leqq \tfrac{1}{4} \tanh^n \tfrac{1}{2}\beta \underset{n\to\infty}{\to} 0 \tag{2.93}$$

because

$$\Lambda_{\max} = 1,$$

and similarly for ρ_n^y.

F. Relationship between Heisenberg and XY Models

It is unfortunately not obvious that the Heisenberg model shows either a stronger or weaker tendency to order than the XY model. On the one hand, one might argue that the Heisenberg model, in which all three components of the spin want to align antiparallel, should show more order than the XY model, in which only two components have this tendency. Equivalently, because the ordering effect of the transverse terms alone in the Heisenberg model is less than that of the transverse terms alone in the XY model, one might conclude that the disordering effect is also correspondingly less in the Heisenberg model. On the other hand, one might argue with perhaps equal justification that the disordering tendency of the transverse terms in the Heisenberg model is greater, there being twice as many such terms. We have so far been unable to show rigorously that either model has a stronger tendency to long-range order than the other.

Lacking a general theorem, it is most interesting for heuristic reasons to consider a simple soluble but nontrivial special case: a chain of six spin $\frac{1}{2}$'s in both the isotropic Heisenberg and isotropic XY models.[7]

For the Heisenberg model a direct diagonalization of the Hamiltonian matrix among the sixty-four possible states is greatly simplified by the knowledge that the ground state is a singlet. It can be further simplified because under reversal of the ordering of the six sites, one of the five singlets of such a chain is even and four (including the ground state) are odd. Diagonalizing the resulting 4×4 matrix, one finds for the ground state

$$\begin{aligned}\Psi_0 = {} & 0.635\,\Phi_{135} - 0.436(\Phi_{136} + \Phi_{235}) - 0.336\,\Phi_{145} \\ & - 0.186(\Phi_{125} + \Phi_{134}) + 0.114(\Phi_{126} + \Phi_{234}) + 0.086\,\Phi_{124} - 0.014\,\Phi_{123}\,,\end{aligned} \tag{2.94}$$

where

$$\Phi_{ijk} = 2^{-\frac{1}{2}}(a_i^\dagger a_j^\dagger a_k^\dagger - a_{6-i}^\dagger a_{6-j}^\dagger a_{6-k}^\dagger)\Phi_0 \tag{2.95}$$

[6] The asymptotic behavior is given by (2.41) with $f(k) \to f(k;\beta) \equiv f(k) \times \tanh \frac{1}{2}\beta\Lambda_k$. It is observed that $f'(0;\beta) = f'(\pi/2;\beta) = 0$ even for $\gamma = 0$, when $\beta \neq 0$ (see footnote 4).

[7] The four-spin problem, though nontrivial, shows too large end effects to be interesting.

and Φ_0 is the state with all spins down.

For the XY model one can specialize the general formalism developed in Section II D to the case $N = 6$. One finds

$$k_m^{\mathrm{I}} = k_m^{\mathrm{II}} = m\pi/7, \tag{2.96}$$

which gives the following G matrix:

$$\mathbf{G} = \begin{pmatrix} 0 & -0.875 & 0 & 0.388 & 0 & -0.300 \\ -0.875 & 0 & -0.485 & 0 & 0.087 & 0 \\ 0 & -0.485 & 0 & -0.774 & 0 & 0.388 \\ 0.388 & 0 & -0.774 & 0 & -0.485 & 0 \\ 0 & 0.087 & 0 & -0.485 & 0 & -0.875 \\ -0.300 & 0 & 0.388 & 0 & -0.875 & 0 \end{pmatrix}. \tag{2.97}$$

The various order parameters may be computed for the Heisenberg model directly from the ground state. ρ_{ij}^z is the simplest to compute; ρ_{ij}^x and ρ_{ij}^y have the same value because Ψ_0 is a singlet. For the XY model the various order parameters may be computed from the appropriate subdeterminants of $\mathbf{G}$. In Table II we exhibit the order parameter ρ_{1j}^x between the first spin and each of the other five. It is immediately clear that the XY model has a stronger tendency to order except for neighboring spins.

The parameter ρ_{1j}^x for the six-spin problem differs from its value when spin $\aleph 1$ is in the middle of an infinite chain because of end effects from both ends. To see the effects of each end for the XY model, we have also tabulated ρ_{1j}^x for a semi-infinite chain (i.e., spin $\aleph 1$ is at one end but the chain is infinitely long) and for an infinite chain (i.e., both the first and jth spins are far from either end). The results for the semi-infinite chain show that the end at the sixth site has a very small effect on the order ρ_{1j}^x; while the results for the infinite chain show that the fact that spin $\aleph 1$ is at an end position has a noticeable but not dominating effect for the six-spin and semi-infinite cases. The results strongly suggest that as $j \to \infty$, ρ_{1j}^x for the semi-infinite and infinite Heisenberg models is dominated by the corresponding parameter for the XY models, which we know

TABLE II

ρ_{1j}^x FOR $j = 2, \ldots, 6$ IN VARIOUS ONE-DIMENSIONAL MODELS

j	2	3	4	5	6
Heis.: 6 spins	−0.222	0.064	−0.077	0.032	−0.047
XY: 6 spins	−0.219	0.106	−0.105	0.065	−0.075
XY: Semi-infinite	−0.212	0.108	−0.102	0.075	−0.077
XY: Infinite	−0.159	0.101	−0.086	0.073	−0.066

TABLE III

$\rho^x_{j,j+1}$ FOR SEVERAL j IN VARIOUS ONE-DIMENSIONAL MODELS

j	1	2	3	∞	$\frac{1}{4}(\rho^x_{12} + 2\rho^x_{23} + \rho^x_{34})$
Heis.:					
6 spins	−0.222	−0.092	−0.202		−0.152
Semi-infinite				−0.148	
XY:					
6 spins	−0.219	−0.121	−0.193		−0.163
Semi-infinite	−0.212	−0.127	−0.182	−0.159	−0.162

tends to zero; i.e., *the isotropic Heisenberg model appears to have vanishing long-range order.*

The end effects on the nearest neighbor order $\rho^x_{j,j+1}$ can also be examined on the basis of values given in Table III. We have exhibited only the cases $j = 1, 2, 3$ because j and $6 - j$ are equivalent for this parameter. We see that for both models the nearest neighbor order oscillates strongly because j is near a free end. However, the effects of the farther end are seen to be small. Furthermore, if the simplest imaginable extrapolation from the six-spin problem is made, a good estimate of the true short-range order in an infinite chain is obtained for both models. Calculations of $\rho^x_{j,j+2}$ and $\rho^x_{j,j+3}$, as well as analogous calculations for the total order parameter, ρ_{ij}, all agree with these conclusions, so they are not exhibited.

III. THE HEISENBERG-ISING MODEL

A. Formulation of Ground-State Problem

The second model consists of $2N$ spin $\frac{1}{2}$'s also arranged in a row and having only nearest neighbor interactions. The interactions are alternately Ising and isotropic Heisenberg interactions, so that the Hamiltonian for a chain with free ends is

$$H_\lambda = \sum_1^N \mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i} + 2\lambda \sum_1^{N-1} S^z_{2i}\mathbf{S}^z_{2i+1} = H_0 + H_1 . \tag{3.1}$$

The parameter λ is to be considered variable but positive and characterizes the relative strength of the two types of interaction.[8]

The particular simplicity of this Hamiltonian is noticed if the representation diagonalizing H_0 is introduced. For the ith pair of spins we introduce the four eigenfunctions of $\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i}$:

[8] The symbol λ is chosen because this parameter appears in many expressions in exactly the same way as does λ for the XY model. In both models, λ ranges from 0 to ∞.

$$\Phi^i_{11} = \uparrow\uparrow, \qquad \Phi^i_{1-1} = \downarrow\downarrow,$$
$$\Phi^i_{10} = \frac{1}{\sqrt{2}}(\downarrow\uparrow + \uparrow\downarrow), \quad \text{and} \quad \Phi^i_{00} = \frac{1}{\sqrt{2}}(\downarrow\uparrow - \uparrow\downarrow); \tag{3.2}$$

where the first and second arrows refer to the $(2i-1)$st and $2i$th spins, respectively, and represent states of a single spin in the positive and negative z-direction. The first subscript of Φ^i refers to the quantum number J_i and the second to M_i for the ith pair. Application of either $S^z_{2i-2}\,S^z_{2i-1}$ or $S^z_{2i}\,S^z_{2i+1}$ to any of these four states leaves the values of M_i unchanged. Thus the assignment of one of the three possible values $(\pm 1, 0)$ to each of the N M_i's defines a subspace of the 2^{2N} dimensional space of all states. The Hamiltonian, having no matrix components between states in different subspaces, can be diagonalized separately in each. It will be shown in Section III E that the ground state is in the subspace for which $M_i = 0$ for all i, a subspace we now consider.

We are faced with a situation that is formally similar to that encountered in the XY model: a set of dynamical systems (in this case a pair of spins) each having two possible states (in this case Φ_{10} and Φ_{00}) and interacting only with the nearest neighbor systems. If we call the states Φ^i_{10} the "up" states and Φ^i_{00} the "down" states, we can formally introduce raising and lowering operators for the ith pair having the usual properties:

$$a_i^\dagger \Phi^i_{00} = \Phi^i_{10}, \qquad a_i^\dagger \Phi^i_{10} = 0, \tag{3.3a}$$

and

$$a_i \Phi^i_{00} = 0, \qquad a_i \Phi^i_{10} = \Phi^i_{00}, \tag{3.3b}$$

so that

$$\{a_i, a_i^\dagger\} = 1 \quad \text{and} \quad a_i^2 = a_i^{\dagger 2} = 0. \tag{3.4}$$

It is to be emphasized that a_i and $a_i^\dagger$ do not lower and raise a particular spin as they did for the XY model. It is only a *formal* analogy between the states Φ^i_{10} and Φ^i_{00} on the one hand, and the up and down orientations of a single spin $\frac{1}{2}$ that we are exploiting.

Because of the fundamental relations

$$S^z_{2i-1}\Phi^i_{10} = -\Phi^i_{00}, \qquad S^z_{2i-1}\Phi^i_{00} = -\Phi^i_{10} \tag{3.5a}$$

and

$$S^z_{2i}\Phi^i_{10} = \Phi^i_{00}, \qquad S^z_{2i}\Phi^i_{00} = \Phi^i_{10}, \tag{3.5b}$$

we may represent S^z_{2i-1} and S^z_{2i} in the $M_i \equiv 0$ subspace by means of a_i and $a_i^\dagger$:

$$S^z_{2i-1} \to -\tfrac{1}{2}(a_i^\dagger + a_i); \qquad S^z_{2i} \to \tfrac{1}{2}(a_i^\dagger + a_i). \tag{3.6}$$

Because the diagonal energies of the states Φ_{10}^i and Φ_{00}^i are, respectively, $\frac{1}{4}$ and $-\frac{3}{4}$, the ith term in H_0 can also be expressed in terms of a_i and $a_i^\dagger$:

$$\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i} \rightarrow a_i^\dagger a_i - \tfrac{3}{4}. \tag{3.7}$$

In the subspace defined by $M_i \equiv 0$, the total Hamiltonian is then

$$H_\lambda = -\tfrac{3}{4}N + \sum_1^N a_i^\dagger a_i - \tfrac{1}{2}\lambda\sum_1^{N-1}(a_i^\dagger + a_i)(a_{i+1}^\dagger + a_{i+1}), \tag{3.8}$$

where, in addition to (3. 4), we have

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = [a_i, a_j^\dagger] = 0. \tag{3.9}$$

The eigenstates and associated energies of H_λ can be found exactly as for the XY model by introducing a complete set of Fermi operators, through (2.5), in terms of which H_λ is given by

$$H_\lambda = -\tfrac{3}{4}N + \sum_1^N c_i^\dagger c_i - \tfrac{1}{2}\lambda\sum_1^{N-1}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}). \tag{3.10}$$

B. Ground State of the Cyclic Chain

It is convenient in this section to consider the "c-cyclic" case obtained by letting $\sum_1^{N-1} \rightarrow \sum_1^N$ in H_1 and defining

$$c_{N+1} \equiv c_1 \quad \text{and} \quad c_{N+1}^\dagger \equiv c_1. \tag{3.11}$$

The matrices relevant to the diagonalization of H_λ are then

$$\mathbf{A} - \mathbf{B} = \begin{pmatrix} 1 & & & -\lambda \\ -\lambda & 1 & 0 & \\ & \ddots & \ddots & \\ & & \ddots & \ddots \\ 0 & & -\lambda & 1 \end{pmatrix} = (\mathbf{A} + \mathbf{B})^T \tag{3.12}$$

and

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \begin{pmatrix} 1+\lambda^2 & -\lambda & & & -\lambda \\ -\lambda & 1+\lambda^2 & -\lambda & 0 & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & 0 & \ddots & \ddots & \ddots \\ -\lambda & & & -\lambda & 1+\lambda^2 \end{pmatrix}. \tag{3.13}$$

For $\lambda \neq 1$ the normal modes are characterized by the functions

$$\phi_{kj} = \begin{cases} (2/N)^{\frac{1}{2}} \sin kj \\ (2/N)^{\frac{1}{2}} \cos kj \end{cases} \tag{3.14a}$$

and

$$\psi_{kj} = \Lambda_k^{-1}[(1 - \lambda \cos k)\phi_{kj} - \lambda \sin k\, \phi_{-kj}], \tag{3.14b}$$

belong to the eigenvalues

$$\Lambda_k = [(1 + \lambda)^2 - 4\lambda \cos^2 \tfrac{1}{2}k]^{\frac{1}{2}}, \tag{3.14c}$$

where

$$k = 2\pi m/N \tag{3.14d}$$

and

$$\begin{aligned} m &= -\tfrac{1}{2}N, \cdots, 0, \cdots, \tfrac{1}{2}N - 1 \quad \text{for } N \text{ even}, \\ m &= -\tfrac{1}{2}(N-1), \cdots, 0, \cdots \tfrac{1}{2}(N-1) \quad \text{for } N \text{ odd}. \end{aligned} \tag{3.14e}$$

We take the upper solution for ϕ_{kj} if $k > 0$, the lower solution if $k \leqq 0$. For $\lambda = 1$ and $m = 0$, we have $\Lambda_k = 0$. For this particular k,

$$\phi_{kj} = N^{-\frac{1}{2}}, \qquad \psi_{kj} = \pm N^{-\frac{1}{2}}. \tag{3.14'}$$

The sign, which is arbitrary, will be taken positive.

It is convenient to introduce the parameter γ, ranging from $+1$ to -1, by

$$\gamma = (1 - \lambda)/(1 + \lambda); \tag{3.15}$$

then

$$\Lambda_k = (1 + \lambda)\,[1 - (1 - \gamma^2)\cos^2 \tfrac{1}{2}\,k]^{\frac{1}{2}}, \tag{3.16}$$

which resembles the spectrum of the XY model.

We see that except for $\lambda = 1$ or $\gamma = 0$ the spectrum of elementary excitations has an energy gap. It should be emphasized, however, that the ground state together with states of all possible combinations of these elementary excitations are but a small subset of the complete set of stationary states, all the rest having one or more $M_i = \pm 1$. Thus, the behavior of the system for finite temperatures is not immediately apparent from the knowledge of the excitation spectrum (3.14c).

The ground-state energy, according to (A-12) is

$$E_0 = -\tfrac{3}{4}N + \tfrac{1}{2}\left(\sum_1^N 1 - \sum_k \Lambda_k\right). \tag{3.17}$$

As $N \to \infty$,

$$E_0/N = -\tfrac{1}{4} - (2/\pi)[1/(1 + \gamma)]\,\mathcal{E}(1 - \gamma^2). \tag{3.18}$$

We notice that E_0/N is not analytic at $\lambda = 1$ ($\gamma = 0$) although it has power

series expansions in λ and $1/\lambda$. This nonanalytic behavior at $\lambda = 1$ is associated with the appearance of long-range order for $\lambda > 1$ as we now show.

C. Short- and Long-Range Order in the Ground State

Define the order parameter in the ground state between pair sites l and m to be

$$\rho_{lm} = \langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m} \mid \Psi_0 \rangle; \tag{3.19}$$

i.e., it is the order between the second spin of each pair. The order between other pairs of spins can be calculated from ρ_{lm} because

$$\langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m-1} \mid \Psi_0 \rangle = - \langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m} \mid \Psi_0 \rangle, \quad \text{etc.} \tag{3.20}$$

Furthermore, the only nonzero contribution to ρ_{lm} is

$$\rho^z_{lm} = \langle \Psi_0 \mid S^z_{2l} S^z_{2m} \mid \Psi_0 \rangle = \tfrac{1}{4} \langle \Psi_0 \mid (a_l^\dagger + a_l)(a_m^\dagger + a_m) \mid \Psi_0 \rangle, \tag{3.21}$$

because S^x_{2l} and S^y_{2l} both change M_l and S^x_{2m} and S^y_{2m} both change M_m. The structure of ρ^z_{lm} is identical with the structure of ρ^x_{lm} for the XY model, so that ρ^z_{lm} is given by the determinant (2.33a) with G_{ij} defined by (2.32c).

For the cyclic chain, $G_{ij} = G_{i-j}$ and in the limit $N \to \infty$ with $r = i - j$ fixed, G_r is found to be given by

$$G_r = (-1)^{r+1} [\tfrac{1}{2}(1 + \gamma) L_{2r}(\gamma) + \tfrac{1}{2}(1 - \gamma) L_{2r+2}(\gamma)], \tag{3.22}$$

where $L_r(\gamma)$ is defined in (2.83b). For the special case of vanishing energy gap, $\lambda = 1$ or $\gamma = 0$,

$$G_r = (2/\pi) [(-1)^{r+1}/(2r + 1)]. \tag{3.23a}$$

For the limiting case of noninteracting Heisenberg pairs,

$$G_r = -\delta_{r0}. \tag{3.23b}$$

In the limit $\lambda \to \infty$ or $\gamma = -1$, which we shall later show to be the Ising limit,

$$G_r = \delta_{r,-1}. \tag{3.23c}$$

In general, for $\lambda \neq 1$,

$$| G_r | < A r^{-4} \quad \text{for} \quad | r | > r_0, \tag{3.24}$$

just as in the XY model.

Hadamard's theorem is sufficient to show that there is no long-range order for $\lambda = 1$, because of the r^{-1} behavior of G_r. For $\lambda \neq 1$, Hadamard's theorem is again too weak, because of the r^{-4} dependence. In the limiting cases $\lambda = 0$ and $\lambda \to \infty$, however, there is no order and perfect order, respectively. This suggests that for $\lambda \leqq 1$ there is no long-range order and for $\lambda > 1$ there is finite long-range

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order, a conjecture that is confirmed for the end-to-end order of a free chain, which we now investigate.

D. End-to-End Order in the Ground State

For a chain of N pairs, the order between the first and last pairs, as in (2.59a) is

$$\rho^z_{1N} = -\tfrac{1}{4}\, G_{N1} \det (\mathbf{A} - \mathbf{B})/ \mid \det (\mathbf{A} - \mathbf{B}) \mid \tag{3.25}$$

providing $\lambda \neq 1$ (to ensure $\Lambda_k \neq 0$). If the chain has free ends,

$$\mathbf{A} - \mathbf{B} = \begin{pmatrix} 1 & & & \mathbf{0} \\ -\lambda & 1 & & \\ & \cdot & \cdot & \\ & & \cdot & \cdot \\ \mathbf{0} & & -\lambda & 1 \end{pmatrix} = (\mathbf{A} + \mathbf{B})^T, \tag{3.26}$$

so that

$$\det (\mathbf{A} - \mathbf{B}) = 1 \quad \text{and} \quad \rho^z_{1N} = -\tfrac{1}{4}\, G_{N1}\,. \tag{3.27}$$

The functions ϕ_{kj} and ψ_{kj} needed to compute G_{N1} are found to be

$$\phi_{kj} = A_k \sin k(N + 1 - j) \quad \text{and} \quad \psi_{kj} = A_k \delta_k \sin kj, \tag{3.28a}$$

where

$$\delta_k = \text{sign of } \sin k/\sin kN. \tag{3.28b}$$

The corresponding eigenvalue is

$$\Lambda_k = [(1 + \lambda)^2 - 4\lambda \cos^2 \tfrac{1}{2}k]^{\frac{1}{2}}, \tag{3.28c}$$

and the normalization constant is

$$A_k = 2\{2N + 1 - [\sin (2N + 1)k]/\sin k\}^{-\frac{1}{2}}. \tag{3.28d}$$

The k's are the roots of

$$\sin k(N + 1)/\sin kn = \lambda. \tag{3.28e}$$

For these k's Λ_k reduces to

$$\Lambda_k = \mid \sin k/\sin Nk \mid. \tag{3.28f}$$

For $\lambda \leqq 1$, there are N real roots, exhausting the normal modes. For $\lambda > 1$, there are $N - 1$ real roots and one imaginary root,

$$k_0 = iv, \tag{3.29}$$

with v defined by

$$\sinh (N + 1)v/\sinh Nv = \lambda. \tag{3.30}$$

For $NV \gg 1$ [i.e., $\lambda - 1 \neq O(1/N)$],

$$e^v = \lambda - [(\lambda^2 - 1)/\lambda](1/\lambda)^{2N}. \tag{3.31}$$

For this particular mode

$$\phi_{k_0 j} = A_{k_0} \sinh (N + 1 - \mathrm{j})v \quad \text{and} \quad \psi_{k_0 j} = A_{k_0} \sinh jv, \tag{3.32a}$$

$$A_{k_0} = 2e^{-Nv}(1 - e^{-2v})^{\frac{1}{2}}, \tag{3.32b}$$

and

$$\Lambda_{k_0} = (\lambda^2 - 1)/\lambda^{N+1}. \tag{3.32c}$$

In evaluating $G_{N1} = -\sum \psi_{kN}\phi_{k1}$, we use the fact (proved in analogy with the XY model, Appendix D) that, except for the mode k_0 and the factor δ_k, the factors in the summand are slowly varying functions of k, and δ_k alternates in sign. Thus

$$G_{N1} = -\psi_{k_0 N}\phi_{k_0 1} + O(1/N) = -(1 - \lambda^{-2}) + O(1/N), \tag{3.33}$$

and

$$\begin{aligned} \rho_{1N} &= \tfrac{1}{4}(1 - \lambda^{-2}) + O(1/N), \qquad \lambda \geqq 1, \\ &= O(1/N), \qquad \lambda < 1. \end{aligned} \tag{3.34}$$

The order in the extremely low-lying excited state with the k_0 excitation present is the same as in the ground state to $O(1/N)$.

E. Excited States

In addition to the excited states produced with the creation operators $\eta_k^\dagger$, there are also all the states lying in subspaces characterized by one or more $M_i \neq 0$. Although it is possible to find states in these subspaces for which each of these M_i is definitely $+1$ or -1, it is much more convenient to work with certain linear combinations of these states. To see why this is, consider the subspace defined by

$$M_1 = 1 \quad \text{and} \quad M_i = 0, \qquad i \neq 1. \tag{3.35}$$

The Hamiltonian in this subspace corresponding to (3.10) is

$$\begin{aligned} H_\lambda = &-\tfrac{3}{4}(N - 1) + \sum_2^N c_i^\dagger c_i \\ &- \tfrac{1}{2}\lambda \sum_2^{N-1} (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - \tfrac{1}{2}\lambda(c_1^\dagger + c_1). \end{aligned} \tag{3.36}$$

Because this Hamiltonian is no longer purely quadratic in the c's and $c^\dagger$'s, it fails to conserve the number of fermions and cannot be diagonalized by a simple principal axis transformation. The difficulty is even greater if the $M = 1$ site is not at the left end, but at $i = p$; for then H_λ is

$$H_\lambda = -\frac{3}{4}(N-1) + \sum_{i\neq p} c_i^\dagger c_i - \frac{1}{2}\lambda \sum_{i\neq p-1,p} (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - \frac{1}{2}\lambda\Big[(c_{p-1}^\dagger - c_{p-1}) \exp\Big(i\pi \sum_1^{p-1} c_j^\dagger c_j\Big) + (c_{p+1}^\dagger + c_{p+1}) \exp\Big(i\pi \sum_1^{p} c_j^\dagger c_j\Big)\Big], \tag{3.36'}$$

which is obviously not directly diagonalizable.

The way around these difficulties is to consider the states with $M_p = \pm 1$ simultaneously, introducing raising and lowering operators $a_p^\dagger$ and a_p which take Φ_{1-1}^p into Φ_{11}^p and vice versa. The Hamiltonian is then a quadratic form in the a's and $a^\dagger$'s (including a_p and $a_p^\dagger$) which remains quadratic, and so is readily diagonalizable, when expressed in the c's and $c^\dagger$'s. The ground state (and all excited states) in this subspace must be doubly degenerate, corresponding to the two linearly independent combinations of Φ_{1-1}^p and Φ_{11}^p, and this must manifest itself in the fact that $\Lambda_k = 0$ for some k. Stationary states with $M_p = \pm 1$ can then be projected from any state if one is so inclined.

Let us consider this procedure more explicitly as generalized to the case of an arbitrary number of sites with $M = \pm 1$. In fact, let

$$|M_i| = 1 \quad \text{for} \quad i = p_1, p_2, \cdots, p_s$$

and (3.37)

$$M_i = 0 \quad \text{for} \quad i \neq p_1, p_2, \cdots, p_s.$$

The pairs at pair sites $p_1, \cdots, p_s$ can be considered as "impurity pairs" embedded in a perfect chain of $M = 0$ pairs. Each set of p's identifies a different subspace and now, because each impurity can also be in two states, all subspaces are still of dimension 2^N.

For an impurity pair at p, we introduce the "up" and "down" states

$$\Phi_+{}^p = \frac{1}{\sqrt{2}}(\Phi_{11}^p + \Phi_{1-1}^p) = \frac{1}{\sqrt{2}}(\uparrow\uparrow + \downarrow\downarrow), \tag{3.38a}$$

$$\Phi_-{}^p = \frac{1}{\sqrt{2}}(\Phi_{11}^p - \Phi_{1-1}^p) = \frac{1}{\sqrt{2}}(\uparrow\uparrow - \downarrow\downarrow), \tag{3.38b}$$

and the raising and lowering operators $a_p^\dagger$ and a_p :

$$a_p^\dagger \Phi_-{}^p = \Phi_+{}^p, \qquad a_p^\dagger \Phi_+{}^p = 0; \tag{3.39a}$$

$$a_p \Phi_-{}^p = 0, \qquad a_p \Phi_+{}^p = \Phi_-{}^p. \tag{3.39b}$$

Because

$$S^z{}_{2p-1}\Phi_+{}^p = S^z{}_{2p}\Phi_+{}^p = \tfrac{1}{2}\Phi_-{}^p \tag{3.40a}$$

and

$$S^z{}_{2p-1}\Phi_-{}^p = S^z{}_{2p}\Phi_-{}^p = \tfrac{1}{2}\Phi_+{}^p, \tag{3.40b}$$

we may represent $S^z{}_{2p-1}$ and $S^z{}_{2p}$ in this subspace by

$$S^z{}_{2p-1} = S^z{}_{2p} = \tfrac{1}{2}(a_p^\dagger + a_p). \tag{3.41}$$

The pth term in H_0 will be simply $\frac{1}{4}$. The interaction of the impurity at p with the $(p-1)$st pair is

$$\tfrac{1}{2}\lambda(a_{p-1}^\dagger + a_{p-1})(a_p^\dagger + a_p), \tag{3.42a}$$

whether the $(p-1)$st pair is an impurity or not. The interaction of the impurity at p with the $(p+1)$st pair is

$$\tfrac{1}{2}\lambda(a_p^\dagger + a_p)(a_{p+1}^\dagger + a_{p+1}) \tag{3.42b}$$

provided $p+1$ is an impurity, and it is

$$-\tfrac{1}{2}\lambda(a_p^\dagger + a_p)(a_{p+1}^\dagger + a_{p+1}) \tag{3.42c}$$

if $p+1$ is not an impurity.

To make all interactions look alike and the same as between two $M = 0$ pairs, it is convenient to introduce new canonical variables in the following way. We make the canonical transformation

$$a_i \to -a_i \quad \text{and} \quad a_i^\dagger \to -a_i^\dagger \tag{3.43}$$

for $p_1 \leqq i < p_2$, $p_3 \leqq i < p_4$, $p_5 \leqq i < p_6$, etc., but leave the other a's and $a^\dagger$'s unchanged. The Hamiltonian in this subspace is then

$$H_\lambda(p_1 \cdots p_s) = -\tfrac{3}{4}N + \varepsilon + \sum_{i \neq p_1, \cdots, p_s} a_i^\dagger a_i - \tfrac{1}{2}\lambda \sum_1^{N-1} (a_i^\dagger + a_i)(a_{i+1}^\dagger + a_{i+1}) \tag{3.44}$$

or simply

$$H_\lambda(p_1 \cdots p_s) = H_\lambda + \sum_{r=1}^{s} (1 - a_{p_i}^\dagger a_{p_i}), \tag{3.44'}$$

where H_λ is the Hamiltonian (3.8) for the case all $M_i = 0$. Although the a's and $a^\dagger$'s on impurity pair sites have a different meaning from the other a's and $a^\dagger$'s, they all have the same formal properties and so (3.44′) is a meaningful statement. It is now clear that the ground state lies in the subspace with no impurities, because if Ψ_0', with energy E_0', is the lowest energy state corresponding to a given set of s impurities, then

$$\left\langle \Psi_0' \middle| \sum_{i=1}^{s} (1 - a_{p_i}^\dagger a_{p_i}) \middle| \Psi_0' \right\rangle = s/2. \tag{3.45}^{9}$$

Thus

$$E_0' = \langle \Psi_0' \mid H_\lambda \mid \Psi_0' \rangle + \tfrac{1}{2}s \geqq E_0 + \tfrac{1}{2}s, \tag{3.46}$$

showing that the ground state has all $M_i = 0$, as previously asserted.

We might mention at this point that, contrary to appearances, we have really included as much anisotropy as is possible, through the variability of λ. An apparent generalization that is still soluble would be to replace H_0 by

$$H_0' = \sum_{1}^{N} [\alpha_1 (S^x{}_{2i-1} S^x{}_{2i} + S^y{}_{2i-1} S^y{}_{2i}) + \alpha_2 S^z{}_{2i-1} S^z{}_{2i}]. \tag{3.47}$$

The corresponding generalization of $H_\lambda(p_1 \cdots p_s)$ is

$$H_\lambda'(p_1 \cdots p_s) = \alpha_1 H_{\lambda/\alpha_1} - \tfrac{1}{4} N(\alpha_2 - \alpha_1) + \tfrac{1}{2}\alpha_2 s + \alpha_1 \sum_{i=1}^{s} (\tfrac{1}{2} - a_{p_i}^\dagger a_{p_i}). \tag{3.48}$$

We see that α_2 has no effect on the stationary states, its only effect being on the energy needed to create impurities. For any $\alpha_2 \geqq 0$, the ground state has no impurities. Only the ratio λ/α_1 has any effect on the wave functions. Thus, without loss of generality, we have chosen $\alpha_1 = \alpha_2 = 1$. Now, provided $\lambda > 0$, this choice of α_2 is exactly equivalent (for the ground-state wave function) to

[9] To prove this, note that the unitary transformation

$$U^{-1} a_{p_i} U = a^\dagger{}_{p_i} \quad \text{and} \quad U^{-1} a^\dagger{}_{p_i} U = a_{p_i} \quad \text{for all } i$$

leaves $H_\lambda(p_1 \cdots p_s)$ unchanged, i.e., $[H_\lambda(p_1 \cdots p_s), U] = 0$. It is thus possible to choose Ψ_0' to be an eigenstate of U as well as of $H_\lambda(p_1 \cdots p_s)$. Then

$$\langle \Psi_0' \mid a_{p_i}^\dagger a_{p_i} \mid \Psi_0' \rangle = \langle U\Psi_0' \mid a_{p_i} a^\dagger{}_{p_i} \mid U\Psi_0' \rangle = \langle \Psi_0' \mid (1 - a^\dagger{}_{p_i} a_{p_i}) \mid \Psi_0' \rangle$$

or

$$\langle \Psi_0' \mid a_{p_i}^\dagger a_{p_i} \mid \Psi_0' \rangle = \tfrac{1}{2} \quad \text{for} \quad i = 1, \cdots, s.$$

the choice $\alpha_2 = 2\lambda$. But with the second choice, $H_\lambda/2\lambda$ becomes the Ising Hamiltonian in the limit $\lambda \to \infty$. Thus the limit $\lambda \to \infty$ is also the Ising limit for the choice $\alpha_2 = \alpha_1 = 1$.

The introduction of impurities at pair sites $p_1, \cdots, p_s$ reduces the matrix $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ into a set of square blocks along the main diagonal of order $p_1, p_2 - p_1, \cdots, N - p_s$, corresponding to the dynamical independence of the different $M = 0$ segments of the chain. Any distribution of impurities can be solved, in principle, because of this independence. The particularly simple distributions of impurities are those in which the first impurity is at the extreme left and the last is at the extreme right, because for such distributions all the nontrivial square blocks have the same structure. It is then convenient to assume the chain has $N + 1$ pair sites and $s + 1$ impurities, the first being at $p_0 = 0$. Then

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \begin{pmatrix} 0 & & & \\ & \mathbf{L}_{q_1} & & \mathbf{0} \\ & & \mathbf{L}_{q_2} & \\ \mathbf{0} & & & \ddots \\ & & & & \mathbf{L}_{q_s} \end{pmatrix}, \tag{3.49}$$

where

$$\mathbf{L}_q = \begin{pmatrix} 1+\lambda^2 & -\lambda & & \mathbf{0} \\ -\lambda & 1+\lambda^2 & -\lambda & \\ & \ddots & \ddots & \ddots \\ & -\lambda & 1+\lambda^2 & \lambda \\ \mathbf{0} & & -\lambda & \lambda^2 \end{pmatrix} \begin{matrix} \\ \\ \\ \\ q \text{ rows and columns} \end{matrix}, \tag{3.50}$$

and $q_i = p_i - p_{i-1}$, the "length" of the ith subchain (including the impurity at the right end, but not the one at the left when the ordering is from left to right).

Let us consider first the case with impurities only at the ends ($p_0 = 0$ and $q_1 = p_1 = N$). One normal mode is

$$\phi_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_0 = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \tag{3.51a}$$

belonging to

$$\Lambda_0 = 0. \tag{3.51b}$$

The other normal modes are

$$\phi_k^{q_1} = A_k^{q_1} \begin{pmatrix} 0 \\ \sin k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_1 k \end{pmatrix} \quad \text{and} \quad \psi_k^{q_1} = -A_k^{q_1}\, \delta_k^{q_1} \begin{pmatrix} \sin q_1 k \\ \cdot \\ \cdot \\ \cdot \\ \sin k \\ 0 \end{pmatrix} \tag{3.52a}$$

with Λ_k given by (3.14c) and

$$\delta_k^{q_1} = \text{sign of } \sin k / \sin (q_1 + 1)k. \tag{3.52b}$$

The k's are the roots of

$$\sin (q_1 + 1)k / \sin q_1 k = 1/\lambda, \tag{3.52c}$$

and so they, and the corresponding Λ_k's, depend on q_1. The excitation of the $\Lambda = 0$ mode corresponds to a reversal of the spins of both impurity pairs and hence of all intervening $M = 0$ pairs, which is why it costs no energy. The two degenerate "ground states" for the chain terminated by two impurity pairs are Ψ_{0-} and Ψ_{0+} defined by

$$\eta_k \Psi_{0-} = 0, \quad \text{all} \quad k, \tag{3.52d}$$

and

$$\eta_k \Psi_{0+} = 0, \qquad k \neq 0 \quad \text{and} \quad \eta_0^{\dagger} \Psi_{0+} = 0. \tag{3.52e}$$

For $\lambda < 1$, there is an imaginary root k_0 of (3.52c) which for $q_1 \to \infty$, has a vanishingly small excitation energy, $\Lambda_{k0} = (\lambda^{-2} - 1)\lambda^{q_1+1}$; but for $\lambda > 1$, there is an energy gap. The creation of the k_0 excitation reverses the relative orientation of the two impurity pairs, as shown in Appendix F. Thus, for $\lambda < 1$ and $q_1 \to \infty$, states with parallel and antiparallel impurity pair alignments have the same energy, a reflection of the absence of long-range order in the intervening $M = 0$ chain. For $\lambda > 1$, on the other hand, the state with antiparallel alignment lies lower in energy by a finite amount, a reflection of the presence of long-range order.

Consider now the same chain but extended to an impurity pair at p_2. In addition to the $\Lambda = 0$ mode, the normal modes are now of two kinds:

$$\Phi_k^{q_1} = A_k^{q_1} \begin{pmatrix} 0 \\ \sin k \\ \sin 2k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_1 k \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad \text{and} \quad \Psi_k^{q_1} = A_k^{q_1}\, \delta_k^{q_1} \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \sin q_1 k \\ \cdot \\ \cdot \\ \cdot \\ \sin 2k \\ \sin k \\ 0 \end{pmatrix}, \tag{3.53}$$

with $\delta_k^{q_1}$ and k defined by (3.52b) and 3.52c); and

$$\Phi_k^{q_2} = A_k^{q_2} \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \sin k \\ \sin 2k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_2 k \end{pmatrix} \quad \text{and} \quad \Psi_k^{q_2} = A_k^{q_2}\, \delta_k^{q_2} \begin{pmatrix} \sin q_2 k \\ \cdot \\ \cdot \\ \cdot \\ \sin 2k \\ \sin k \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}, \tag{3.54}$$

with $\delta_k^{q_2}$ and k defined by the analogs of (3.52b) and (3.52c). Arguments similar to those in Appendix F can be used to show that in the lowest state, successive impurity pairs are aligned antiparallel. Any odd number of excitations of the left segment results in a parallel alignment of impurity pairs at p_0 and p_1; and similarly odd numbers of excitations of the right segment result in parallel alignment of pair sites p_1 and p_2. If $\lambda < 1$, and p_1 is far from one end, the k_0 excitation of this long segment gives the corresponding parallel alignment at a negligible cost of energy. But if $\lambda > 1$, these parallel alignments cost finite amounts of energy, a consequence of the long-range order.

The above discussion is obviously generalizable immediately to any number of impurities. For a chain of length $N + 1$, the lowest energy in a subspace characterized by the impurity pairs at $p_0 = 0, p_1, \cdots, p_{s-1}, p_s = N$, or by the chain segments $q_1, \cdots, q_s, \sum_1^s q_r = N$ is

$$E_0(q_1, \cdots, q_s) = -\frac{1}{4}(N-1) + \frac{1}{2}\sum_{r=1}^{s}\left[1 - \sum_{k(q_r)} \Lambda_k\right]. \tag{3.55}$$

The quantity $\frac{1}{2}[1 - \sum_{k(q)} \Lambda_k] \equiv \mathcal{U}(q)$ can be simply interpreted as the sum of the self-energy of an impurity embedded in an $M = 0$ chain and the interaction energy of this impurity with another one, q pair sites away. It can be more simply regarded, however, just as the energy of a chain segment (with an impurity at the right end) of length q; the entire chain is then a collection of noninteracting segments, arbitrary in number, obeying only the constraint $\sum_1^s q_r = N$.

F. Statistical Mechanics

To evaluate the partition sum of the Heisenberg–Ising model, we first evaluate it for all the internal degrees of freedom in each segment, which leads to a temperature dependent $\mathcal{U}(q)$:

$$\exp\,[-\beta\mathcal{U}(q;\beta)] \equiv \prod_{k(q)} (1 + \exp(-\beta\Lambda_k)). \tag{3.56}$$

We then sum over all configurations of $s - 1$ internal impurities and then sum over s:

$$Z_N(\beta) = \sum_s \sum_{\substack{q_1,\cdots q_r \\ \Sigma q_r = N}} \exp\left[-\beta \sum_{r=1}^{s} \mathcal{U}(q_r\,;\beta)\right] \tag{3.57}$$

It is appealing to handle the constraint $\sum q_r = N$ in analogy with the grand canonical ensemble, but because the exact free energy increases linearly with N for large N, such a method fails. Rather the constraint can be introduced explicitly using the integral representation for the Kronecker delta:

$$\delta_{\Sigma q,N} = (1/2\pi) \int_{-\pi}^{\pi} \exp[i\theta(\textstyle\sum q - N)]d\theta. \tag{3.58}$$

Then

$$Z_N(\beta) = \sum_s \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp(-i\theta N)[z(\theta;\beta)]^s = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \frac{\exp(-i\theta N)}{1 - z(\theta;\beta)}, \tag{3.59}$$

where

$$z(\theta;\beta) = \sum_{q=1}^{\infty} \exp[-\beta\mathcal{U}(q;\beta) + i\theta q]. \tag{3.60}$$

This reduces the problem to quadratures, which we shall not carry out.

G. The Approximation of Ruijgrok and Rodriguez

It is interesting to consider the most successful of the approximate procedures for the Heisenberg model, that of Ruijgrok and Rodriguez (*10*), (henceforth, RR), to see how accurately it gives the various properties of the Heisenberg–

Ising (HI) model that are known exactly. The procedure of RR is to introduce operators ξ_k and $\xi_k^\dagger$ similar to η_k and $\eta_k^\dagger$ of the XY model, operators that annihilate or create particles (i.e., spins up) in Bloch wave single particle states with two sites per unit cell rather than in plane wave single particle states as we did for the cyclic isotropic XY model. The best form for the Bloch waves is determined variationally. Thus their method gives the isotropic XY model exactly (the Bloch waves reduce to plane waves), but it is not really suited to the anisotropic XY model because the latter fails to conserve the number of particles, whereas the RR method is particle conserving. The Heisenberg–Ising model, on the other hand, is also particle conserving, if by particles we mean single up-spins, not to be confused with up and down pair states. Furthermore, the HI Hamiltonian is invariant under translations by an even number of spin sites, providing it is made suitably cyclic. It is thus appropriate for a test of the RR procedure.

The cyclic HI-Hamiltonian in terns of the c's and $c^\dagger$'s introduced in (2.5a, b) is

$$H_\lambda = \sum_{j=1.3\cdots}^{2N-1} [(c_j^\dagger c_j - \tfrac{1}{2})(c_{j+1}^\dagger c_{j+1} - \tfrac{1}{2}) + \tfrac{1}{2}(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger)] + 2\lambda \sum_{j=2,4\cdots}^{2N} (c_j^\dagger c_j - \tfrac{1}{2})(c_{j+1}^\dagger c_{j+1} - \tfrac{1}{2}). \tag{3.61}$$

Following RR, operators ξ_k and $\xi_k^\dagger$ are introduced to diagonalize H approximately:

$$\xi_k = \sum_j e^{ikj} u_k(j) c_j = (\xi_k^\dagger)^\dagger \tag{3.62}$$

with

$$u_k(j) = (2N)^{-\frac{1}{2}} [\cos \alpha(k) + (-1)^j \sin \alpha(k)]. \tag{3.63}$$

TABLE IV

COMPARISON OF THE RUIJGROK–RODRIGUEZ APPROXIMATE LONG-RANGE ORDER IN THE GROUND STATE OF THE HI MODEL WITH THE CORRESPONDING EXACT VALUES FOR VARIOUS VALUES OF λ

λ	0	½	1	2.5	5
E_{RR}/N	−0.485	−0.615	−0.829	−1.541	−2.771
E_0/N	−0.750	−0.782	−0.887	−1.550	−2.775
$\rho_\infty{}^z$,RR	0.057	0.162	0.202	.234	.245
$\rho_\infty{}^z$ exact	0.000	0.000	0.000	.210	.240

The function $\alpha(k)$ is chosen to minimize the expectation value of H_λ in the Fermi sea of ξ-particles. The energy per spin is found to be

$$E_{RR}/N = [1/4(1 + 2\lambda)] - [(1 + 2\lambda)/\pi^2]\mathfrak{K}^2(\mu^2), \tag{3.64}$$

where μ is the solution of the transcendental equation

$$\mu\mathfrak{D}(\mu^2) = \pi/2(1 + 2\lambda). \tag{3.65}$$

$\mathfrak{K}$ and $\mathfrak{D}$ are again complete elliptical integrals. In Table IV we compare the energy per spin and long-range order calculated for the RR approximate ground state with the exact energy per spin and end-to-end order, for several values of λ. We see that although the RR procedure gives the asymptotically correct energy as $\lambda \to \infty$, and a good approximation to the energy for $\lambda > 1$, it may give the order quite incorrectly. This emphasizes the danger of relying on a variational approach for the long-range order, a result which is not surprising in view of the fact that states with no long-range order can be constructed with energy/spin above the ground state by only $O(N^{-2})$.

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APPENDIX A. TO DIAGONALIZE A GENERAL QUADRATIC FORM IN FERMI OPERATORS

We wish to diagonalize the quadratic form

$$H = \sum_{i,j} [c_i^\dagger A_{ij} c_j + \tfrac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.})], \tag{A-1}$$

where the c_i's and $c_i^\dagger$'s are Fermi annihilation and creation operators and H is Hermitian. The Hermiticity of H requires that **A** be a Hermitian matrix, while the anticommutation rules among the c_i's require that **B** be an antisymmetric matrix. In the situations of interest *here*, one can always arrange that **A** and **B** are real.

We try to find a linear transformation of the form

$$\eta_k = \sum_i (g_{ki} c_i + h_{ki} c_i^\dagger), \tag{A-2a}$$

$$\eta_k^\dagger = \sum_i (g_{ki} c_i^\dagger + h_{ki} c_i), \tag{A-2b}$$

with the g_{ki} and h_{ki} real, which is canonical (i.e., the η_k's and $\eta_k^\dagger$'s should also be Fermi operators) and which gives for H the form

$$H = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \text{constant}. \tag{A-3}$$

If this is possible, then

$$[\eta_k, H] - \Lambda_k \eta_k = 0. \tag{A-4}$$

Substituting (A-2) in (A-4) and setting the coefficients of each operator equal to zero, we obtain a set of equations for the g_{ki} and h_{ki} :

$$\Lambda_k g_{ki} = \sum_j (g_{kj} A_{ji} - h_{kj} B_{ji}), \tag{A-5a}$$

$$\Lambda_k h_{ki} = \sum_j (g_{kj} B_{ji} - h_{kj} A_{ji}). \tag{A-5b}$$

These are simplified by introducing the linear combinations

$$\phi_{ki} = g_{ki} + h_{ki} \tag{A-6a}$$

and

$$\psi_{ki} = g_{ki} - h_{ki} \tag{A-6b}$$

in terms of which the coupled equations are

$$\phi_k(\mathbf{A} - \mathbf{B}) = \Lambda_k \psi_k \tag{A-7a}$$

and

$$\psi_k(\mathbf{A} + \mathbf{B}) = \Lambda_k \phi_k \tag{A-7b}$$

in an obvious matrix notation. Either ψ_k or ϕ_k can be eliminated from (A-7) giving either

$$\phi_k(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \Lambda_k^2 \phi_k \tag{A-8a}$$

or

$$\psi_k(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) = \Lambda_k^2 \psi_k . \tag{A-8b}$$

For $\Lambda_k \neq 0$, either (A-8a) or (A-8b) is solved for ϕ_k or ψ_k and the other vector is then obtained from (A-7a) or (A-7b).

For $\Lambda_k = 0$, both ϕ_k and ψ_k are determined by (A-8), or more simply by (A-7), their relative sign being arbitrary. Changing the sign of ψ_k , but not of ϕ_k , interchanges g_{kj} and h_{kj} , hence η_k and $\eta_k^\dagger$, and thus interchanges the definitions of occupied and unoccupied for this zero-energy mode. That the choice of definition is arbitrary is not surprising, because it has no effect on the energy.

Because $\mathbf{A}$ is symmetric and $\mathbf{B}$ is antisymmetric, $(\mathbf{A} + \mathbf{B})^T = \mathbf{A} - \mathbf{B}$, so that both $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ and $(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})$ are symmetric and at least positive semi-definite. Thus all the Λ_k's are real and it is possible to choose all the ϕ_k's and ψ_k's to be real as well as orthogonal. If the ϕ_k's are normalized

vectors ($\sum_i \phi_{ki}^2 = 1$), then the ψ_k's are also automatically normalized when $\Lambda_k \neq 0$ or can be so chosen when $\Lambda_k = 0$. This ensures that

$$\sum_i (g_{ki}g_{k'i} + h_{ki}h_{k'i}) = \delta_{kk'} \tag{A-9a}$$

and

$$\sum_i (g_{ki}h_{k'i} - g_{k'i}h_{ki}) = 0, \tag{A-9b}$$

the necessary and sufficient conditions that the η_k's and $\eta_k^\dagger$'s be canonical Fermi operators.

The constant in H can be determined by substituting (A-3) in (A-1) or, less tediously, from the invariance of tr H under the canonical transformation (A-2). From (A-1)

$$\text{tr } H = 2^{N-1} \sum_i A_{ii} \tag{A-10}$$

while from (A-3)

$$\text{tr } H = 2^{N-1} \sum_k \Lambda_k + 2^N \times \text{constant}. \tag{A-11}$$

The constant is thus $\frac{1}{2}(\sum_i A_{ii} - \sum_k \Lambda_k)$ and

$$H = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \frac{1}{2}\left(\sum_i A_{ii} - \sum_k \Lambda_k\right). \tag{A-12}$$

APPENDIX B. NONDEGENERACY OF THE GROUND STATE AND ABSENCE OF AN ENERGY GAP IN THE HEISENBERG MODEL

We prove two exact theorems about the ground state and excitation spectrum for a Heisenberg model with nearest neighbor interactions in one dimension. The generalization to longer range interactions and higher-dimensional lattices is indicated. A further generalization to particles of spin $\neq \frac{1}{2}$ and a discussion of the ordering of excited state energy levels has been submitted for publication in the *Journal of Mathematical Physics* by Lieb and Mattis.

THEOREM 1. For a linear chain of spin $\frac{1}{2}$'s with nearest neighbor antiferromagnetic Heisenberg interactions, the ground state is nondegenerate (hence $S = 0$).

Proof. We first remark that this is a stronger theorem than that due to Marshall (7), who proved that there is a singlet ground state, but who did not exclude the possibility of there being several degenerate ground states, some of which may not be singlets. We consider the Hamiltonian

$$H = \sum S^z{}_i S^z{}_j + \tfrac{1}{2}\sum S^+{}_i S^-{}_j + S^-{}_i S^+{}_j, \tag{B-1}$$

where i and j are on the A and B sublattices respectively and the sums run over all interacting pairs. It is convenient to make the canonical transformation rotating all spins on the B sublattice ($S^x_j \to -S^x_j$, $S^y_j \to -S^y_j$, $S^z_j \to S^z_j$), so that instead of (B-1) we consider

$$H' = \sum S^z_i S^z_j - \tfrac{1}{2}\sum S^+_i S^-_j + S^-_i S^+_j . \tag{B-2}$$

Because $[S_z, H] = 0$, let us consider only states having $S_z = 0$ and show that only one such state has the ground-state energy. A complete set of states in the $S_z = 0$ subspace is the set of configurations in which $N/2$ spins are up and $N/2$ spins are down. We denote these states by Φ_μ where $1 \leqq \mu \leqq \binom{N}{\frac{1}{2}N}$. Any eigenfunction Ψ of H' can be expanded as

$$\Psi = \sum C_\mu \Phi_\mu , \tag{B-3}$$

and Schrödinger's equation in this representation reduces to a set of coupled linear equations

$$(E - \epsilon_\mu) C_\mu = \tfrac{1}{2} \sum_{\mu' (\mu)} C_{\mu'} , \tag{B-4}$$

where

$$\epsilon_\mu \Phi_\mu = (\sum S^z_i S^z_j)\Phi_\mu ,$$

and the $\Phi_{\mu'(\mu)}$ are the set of configurations which connect to Φ_μ via the interaction. Because the Hamiltonian is real, we may assume without loss of generality that all C's are real. Essential to the proof is the following lemma:

LEMMA 1. For any ground state with $S_z = 0$, all $C_\mu \neq 0$.

Proof. Suppose the contrary, i.e., for some ground state Ψ_0 having the ground-state energy E_0,

$$C_\mu = 0 \quad \text{for} \quad \mu = \mu_1 , \cdots , \mu_r . \tag{B-5a}$$

For these C's (B-2) reduces to

$$0 = \tfrac{1}{2} \sum_{\mu\ (\mu)} C_{\mu'}, \qquad \mu = \mu_1 , \cdots , \mu_r . \tag{B-5b}$$

Now in at least one of these equations, say the μ_pth, some of the $C_{\mu'}$'s $\neq 0$ (otherwise H would break into blocks with no matrix elements connecting $\Phi_{\mu_1} , \cdots , \Phi_{\mu_r}$ with the other configurations, which is readily seen to be impossible); therefore (B-5b) implies that there are nonzero C's of *both* signs. Consider then the trial function Ψ_0':

$$\Psi_0' = \sum | C_\mu | \Phi_\mu . \tag{B-6}$$

On the one hand, Ψ_0' is not an eigenstate because

$$| C_{\mu_p} | = 0 \quad \text{but} \quad \sum_{\mu \, (\mu_p)} | C_{\mu'} | \neq 0, \tag{B-7}$$

so that, from the variational principle, we have for its energy

$$E_0' > E_0 . \tag{B-8}$$

On the other hand, explicit evaluation gives

$$E_0' = \sum \epsilon_\mu C_\mu^2 - \tfrac{1}{2} \sum_{\mu} \sum_{\mu'(\mu)} | C_\mu | \, | C_{\mu'} | \tag{B-9a}$$

and

$$E_0 = \sum \epsilon_\mu C_\mu^2 - \tfrac{1}{2} \sum_{\mu} \sum_{\mu'(\mu)} C_\mu C_{\mu'} , \tag{B-9b}$$

from which it follows that

$$E_0' \leqq E_0 . \tag{B-10}$$

The contradiction between (B-8) and (B-10) proves the lemma.

We now prove a lemma which is a stronger version of the lemma due to Peierls and used by Marshall.

LEMMA 2. For every ground state with $S_z = 0$, all C_μ's have the same sign.

Proof. For Ψ_0 to be a ground state, the equality must hold in (B-10). This occurs if, and only if, all the terms $C_\mu C_{\mu'}$ occuring in (B-9b) are positive, (they are all nonzero by lemma 1), i.e., the coefficients of all configurations connected through the interaction with each other should have the same sign. But as we have remarked, each configuration is ultimately connected with every other through repeated applications of the interaction, proving the lemma.

It is now obvious that there can be only one ground state with $S_z = 0$; otherwise, the several states would all have all positive coefficients and so could not be orthogonal to one another. Now Marshall has shown that *at least* one ground state has $S = 0$. The existence of another ground state, whatever its multiplicity, would imply that there is a second ground state with $S_z = 0$, which we have shown to be impossible. The entire proof is immediately generalizable to any number of dimensions and any lattice which is decomposable into two equivalent sublattices with antiferromagnetic Heisenberg interactions between spins on different sublattices and ferromagnetic Heisenberg interactions between spins on the same sublattice. Also, although Marshall's proof, used above, requires periodic boundary conditions to ensure translational invariance, this restriction may also be dropped if the lattice has reflection symmetry about some plane (so that there is a transformation mapping the A and B sublattices into each other but leaving the Hamiltonian unchanged).

Next we investigate the nature of the excitation spectrum and prove

THEOREM 2. There is an excited state for the cyclic linear chain with nearest neighbor Heisenberg interactions having vanishingly small excitation energy in the limit that the length of the chain becomes infinite.

Proof. Consider the state

$$\Psi_k = \exp\,(ik\sum nS^z{}_n)\Psi_0 \equiv \mathcal{O}^k\Psi_0\,. \tag{B-11}$$

We first show that if $k = (2\pi/N) \times$ odd integer, Ψ_k is orthogonal to the ground state. Consider the unitary operator U_x that displaces all the spins by one site cyclically:

$$U_x\mathbf{S}_iU_x^{-1} = \mathbf{S}_{i+1}\,, \qquad \mathbf{S}_{N+1} = \mathbf{S}_1\,. \tag{B-12}$$

Because

$$[H,U_x] = 0,$$

if Ψ_0 is an eigenstate of H, so is $U_x\Psi_0$. By the nondegeneracy of Ψ_0

$$U_x\Psi_0 = e^{i\alpha}\Psi_0\,. \tag{B-13}$$

Thus

$$\begin{aligned}\langle\Psi_0 \mid \Psi_k\rangle &= \langle\Psi_0 \mid \mathcal{O}^k \mid \Psi_0\rangle \\ &= \langle\Psi_0 \mid U_x\mathcal{O}^kU_x^{-1} \mid \Psi_0\rangle.\end{aligned} \tag{B-14}$$

But

$$U_x\mathcal{O}^kU_x^{-1} = \mathcal{O}^k \exp\,(ikNS^z{}_1) \exp\,(-ik\sum_1^N S^z{}_n). \tag{B-15}$$

Because Ψ_0 is a singlet

$$\exp\,(-ik\sum_1^N S^z{}_n)\Psi_0 = 0. \tag{B-16}$$

Furthermore, in the most convenient representation

$$S^z{}_1 = \begin{pmatrix} \tfrac{1}{2} & 0 \\ 0 & -\tfrac{1}{2} \end{pmatrix} \tag{B-17a}$$

so that

$$\exp(ikNS^z{}_1) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tag{B-17b}$$

in this or any other representation, providing

$$k = 2\pi m/N, \quad m \text{ an odd integer.} \tag{B-18}$$

Thus

$$\langle \Psi_0 \mid \Psi_k \rangle = -\langle \Psi_0 \mid \Psi_k \rangle = 0. \tag{B-19}$$

Note that we have not proved the Ψ_k's to be orthogonal among themselves. The energy of Ψ_k is also readily calculated.

$$\langle \Psi_k \mid H \mid \Psi_k \rangle = \langle \Psi_0 \mid \mathcal{O}_x^{k-1} H \mathcal{O}^k \mid \Psi_0 \rangle. \tag{B-20}$$

Using,

$$\mathcal{O}^{k-1} S^x{}_n \mathcal{O}^k = S^x{}_n \cos kn + S^y{}_n \sin kn, \tag{B-21a}$$

$$\mathcal{O}^{k-1} S^y{}_n \mathcal{O}^k = -S^x{}_n \sin kn + S^y{}_n \cos kn, \tag{B-21b}$$

and

$$\mathcal{O}^{k-1} S^z{}_n \mathcal{O}^k = S^z{}_n , \tag{B-21c}$$

we find

$$\langle \Psi_0 \mid \mathcal{O}^{k-1} H \mathcal{O}^k \mid \Psi_0 \rangle = \Big\langle \Psi_0 \Big| H + (\cos k - 1) \sum_1^N (S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1}) + \sin k \sum_1^N (S^x{}_n S^y{}_{n+1} - S^y{}_n S^x{}_{n+1}) \Big| \Psi_0 \Big\rangle. \tag{B-22}$$

Use has been made of (B-18) in the term arising from $\mathbf{S}_N \cdot \mathbf{S}_1$. Consider the terms on the right in (B-22), one by one, for $k = 2\pi/N$.

(i) $$\langle \Psi_0 \mid H \mid \Psi_0 \rangle = E_0 . \tag{B-23a}$$

(ii) $$(\cos k - 1) \Big\langle \Psi_0 \Big| \sum_1^N (S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1}) \Big| \Psi_0 \Big\rangle$$

$$= \left[-\tfrac{1}{2} \left(\frac{2\pi}{N} \right)^2 - O(N^{-4}) \right] \sum_1^N \langle \Psi_0 \mid S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1} \mid \Psi_0 \rangle \tag{B-23b}$$

$$\leq \left(\frac{2\pi}{N} \right)^2 \frac{N}{2} + O(N^{-3}).$$

(iii) $$\sin k \Big\langle \Psi_0 \Big| \sum_1^N (S^x{}_n S^y{}_{n+1} - S^y{}_n S^x{}_{n+1}) \Big| \Psi_0 \Big\rangle = -i \sin k \, \langle \Psi_0 \mid [\textstyle\sum n S^z{}_n , H] \mid \Psi_0 \rangle = 0. \tag{B-23c}$$

Thus for $k = 2\pi/N$,

$$\langle \Psi_k \mid H \mid \Psi_k \rangle \leqq E_0 + (2\pi^2/N), \tag{B-24}$$

and there is no energy gap.

In two dimensions we consider a square lattice of N sites in the x-direction and of $M = O(N^\nu)$ sites in the y-direction, where $0 < \nu < 1$. The Hamiltonian is assumed cyclic in the sense that

$$\mathbf{S}_{n,\,M+1} = \mathbf{S}_{n,\,1} \tag{B-25a}$$

and

$$\mathbf{S}_{N+1,\,m} = \mathbf{S}_{1,\,m}\,, \tag{B-26}$$

i.e., the lattice is wrapped on a torus. We take for the operator $\mathcal{O}^k$,

$$\mathcal{O}^k = \exp\left(ik \sum_{n=1}^{N} \sum_{m=1}^{M} n S^z{}_{n,m}\right). \tag{B-27}$$

This operator twists the direction of all spins with the same x-coordinate by the same amount. Ψ_k is constructed and its orthogonality to the ground state is proved precisely as in one dimension. Instead of (B-24), one now has

$$\langle \Psi_k \mid H \mid \Psi_k \rangle \leqq E_0 + (2\pi^2/N^{1-\nu}); \tag{B-28}$$

so again there is no energy gap. Because the excitation energy of exact low-lying states should not depend on the shape of the entire lattice, there should be no energy gap for a lattice of $N \times N$ sites either. The particular state Ψ_k is unfortunately not sufficiently like an exact low-lying excited state to give this result.

A similar extension to three dimensions is obvious.

APPENDIX C. CALCULATING $G_{ij}(\beta)$ FOR THE XY MODEL

By definition

$$G_{ij} = \langle B_i A_j \rangle. \tag{C-1}$$

In the ground state

$$G_{ij} = \langle \Psi_0 \mid B_i A_j \mid \Psi_0 \rangle \tag{C-2a}$$

while at finite temperature

$$G_{ij} = \langle B_i A_j \rangle_\beta\,,$$

where $\langle \ldots \rangle_\beta$ denotes an average over the canonical ensemble at temperature $T = 1/k$. Thus

$$\begin{aligned} G_{ij}(\beta) &= \sum_{kk'} \psi_{ki}\phi_{k'j} \langle (\eta_k^\dagger - \eta_k)(\eta_{k'}^\dagger + \eta_{k'}) \rangle_\beta \\ &= \sum_k \psi_{ki}\phi_{kj} (\langle \eta_k^\dagger \eta_k \rangle_\beta - \langle \eta_k \eta_k^\dagger \rangle_\beta). \end{aligned} \tag{C-3}$$

But

$$\langle \eta_k^\dagger \eta_k \rangle = [\exp(\beta\Lambda_k) + 1]^{-1}, \text{ etc.},$$

so that

$$G_{ij}(\beta) = -\sum_k \psi_{ki}\phi_{kj} \tanh(\tfrac{1}{2}\beta\Lambda_k) = -(\psi^T \tanh(\tfrac{1}{2}\beta\Lambda)\phi)_{ij}. \quad \text{(C-4)}$$

For the cyclic chain, the sum in (C-4) can be considerably simplified. First, combining the summands for k and $-k$,

$$G_{ij}(\beta) = -(2/N)\sum_{k>0} \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cdot[\cos k \cos k(i-j) - \gamma \sin k \sin k(i-j)]. \quad \text{(C-5)}$$

Second, combining the summands for k and $\pi - k$,

$$G_{ij}(\beta) = -(4/N)\frac{1-(-1)^{i-j}}{2} \sum_{0<k<\pi/2} \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cdot[\cos k \cos k(i-j) - \gamma \sin k \sin k(i-j)]. \quad \text{(C-6)}$$

For $N \to \infty$ with $i - j = r$ fixed,

$$G_r = -\left[\frac{1+\gamma}{2} L_{r+1} + \frac{1-\gamma}{2} L_{r-1}\right], \qquad r \text{ odd}$$

$$G_r = 0, \qquad r \text{ even}, \quad \text{(C-7)}$$

where

$$L_r = (2/\pi)\int_0^{\pi/2} dk \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cos kr. \quad \text{(C-8)}$$

G_r for the ground state is obtained by setting $\tanh(\tfrac{1}{2}\beta\Lambda_k) \equiv 1$.

APPENDIX D. DEPENDENCE OF $\sin^2 Nk$ AND A_k^2 ON k FOR A CHAIN WITH FREE ENDS, XY MODEL

In this appendix we wish to show that for a chain with free ends, A_k^2 and $\sin^2 Nk$ are smoothly varying functions of k in the sense that the change in either of them when k_m is replaced by k_{m+1} is $O(1/N)$ (except when k_{m+1} is k_0, the bound state).

First consider $\sin^2 Nk$.

$$\Delta \sin^2 Nk_m = \tfrac{1}{2}(\cos 2Nk_m - \cos 2Nk_{m+1}) = \tfrac{1}{2}(\cos 2\nu_m\pi - \cos 2\nu_{m+1}\pi). \quad \text{(D-1)}$$

But because ν_m is obviously a slowly varying function of m, from (2.67′) or (2.69), we have

$$\Delta \sin^2 Nk_m = \pi \sin 2\nu_m \pi \, \Delta\nu_m = O(1/N). \tag{D-2}$$

Second, consider A_k. Letting

$$\chi_m = \sin 2(N+1)k_m / \sin 2k_m ,$$

we have

$$\Delta A_{k_m}^2 \equiv A_{k_{m+1}}^2 - A_{k_m}^2 = 4(N + 1 - \chi_m)^{-2} \, \Delta\chi_m \tag{D-3}$$

providing

$$\Delta\chi_m/(N + 1 - \chi_m) \ll 1. \tag{D-4}$$

Now, as $N \to \infty$,

$$\chi_m = \frac{\sin[(2m/N) - \nu_m]\pi}{\sin(2m\pi/N)} = \cos \nu_m \pi - \cot \frac{2m\pi}{N} \sin \nu_m \pi \tag{D-5}$$

and

$$\begin{aligned}\Delta\chi_m = {} & -[\sin \nu_m\pi + \cot(2m\pi/N) \cos \nu_m\pi]\pi\Delta\nu_m \\ & - \sin \nu_m\pi \, \Delta\cot(2m\pi/N).\end{aligned} \tag{D-6}$$

For $\frac{1}{2}N - m = O(N)$, these relations give

$$\chi_m = O(1) \quad \text{and} \quad \Delta\chi_m = O(1/N), \tag{D-7}$$

so that (D-4) is satisfied and (D-3) gives

$$\Delta A_{k_m}^2 = O(1/N^3). \tag{D-8}$$

For $\frac{1}{2}N - m \equiv m' = o(N) \neq 0$, one must be more careful. Then

$$\Delta A_{k_m}^2 = 4\Delta\chi_m/(N + 1 - \chi_{m+1})(N + 1 - \chi_m). \tag{D-9}$$

In this limit

$$\chi_m = \cos \nu_m\pi + (N/2m'\pi) \sin \nu_m\pi = (N/2m'\pi) \sin \nu_m\pi + o(N). \tag{D-10}$$

Thus

$$\Delta\chi_m = (N/2\pi) \, [\sin \nu_m\pi/m'(m' - 1)] + o(N), \tag{D-11}$$

so that

$$\Delta A_{k_m}^2 = O(1/N). \tag{D-12}$$

APPENDIX E. G_{ij} FOR THE XY MODEL WITH FREE ENDS

In this appendix we derive simple relations between G^f_{ij} for the XY model with free ends and G^c_{i-j} for the cyclic XY model, valid except when i and j are near opposite ends.

In general

$$G_{ij} = -\sum_k \psi_{ki}\phi_{kj}\,. \tag{E-1}$$

For free ends, the sum on k is over modes of Type I and Type II. If i is odd $\psi^{\mathrm{II}}_{ki} = 0$ so that only Type I modes contribute; but for Type I modes, $\phi^{\mathrm{I}}_{kj} = 0$ unless j is even. Thus

$$G^f_{ij} = -\sum_{k^{\mathrm{I}}} \psi^{\mathrm{I}}_{ki}\phi^{\mathrm{I}}_{kj} = \sum_{k^{\mathrm{I}}} A_k{}^2\delta_k \sin[(N-i+1)k]\sin jk \quad \text{for } i \text{ odd}, j \text{ even}; \tag{E-2a}$$

similarly,

$$G^f_{ij} = \sum_{k^{\mathrm{II}}} A_k{}^2\delta_k \sin ik \sin[(N+1-j)k] \quad \text{for } i \text{ even}, j \text{ odd}; \tag{E-2b}$$

and finally,

$$G^f_{ij} = 0 \quad \text{for } i \text{ and } j \text{ both even or both odd.} \tag{E-2c}$$

Furthermore, $k_{\mathrm{I}} \leftrightarrow k_{\mathrm{II}}$ is equivalent to $\gamma \to -\gamma$, so that

$$G^f_{ij}(\gamma) = G^f_{ji}(-\gamma), \tag{E-3a}$$

and for the cyclic chain we have a similar relation

$$G^c_{i-j}(\gamma) = G^c_{j-i}(-\gamma). \tag{E-3b}$$

Therefore we need consider only the case i odd and j even.

Defining

$$r = i - j, \tag{E-4a}$$

$$s = i + j, \tag{E-4b}$$

we obtain

$$G^f_{ij} = \tfrac{1}{2}\sum_{k^{\mathrm{I}}} A_k{}^2\delta_k[\cos(N+1-s)k - \cos(N+1-r)k], \tag{E-5}$$

and we have two sums on the right of identical structure. Suppose first that $s = o(N)$. Then using (2.66) and neglecting terms of $O(1/N)$ we find

$$\cos(N+1-s)k_m{}^{\mathrm{I}} = (-1)\cos\{\nu_m{}^{\mathrm{I}} - [(1-s)m/N]\}\pi. \tag{E-6}$$

From (2.67′) it follows immediately that

$$\tfrac{1}{2} \sum_{k\mathrm{I}} A_k^2 \delta_k \cos\,(N + 1 - s)k = -G_s^c \tag{E-7}$$

so that

$$G_{ij}^f = G_{i-j}^c - G_{i+j}^c \quad \text{for} \quad i \text{ odd}, j \text{ even}, \mid i - j \mid = o(N), \quad \text{and} \quad i + j = o(N). \tag{E-8a}$$

From (E-3a, b) we have also

$$G_{ij}^f = G_{i-j}^c - G_{-(i+j)}^c \quad \text{for} \quad i \text{ even}, j \text{ odd}, \mid i - j \mid = o(N) \quad \text{and} \quad i + j = o(N). \tag{E-8b}$$

If both i and j are far from the ends but not far from each other, we suppose $r = o(N)$ but $s = \sigma N$ where $\sigma = O(1)$. Then, using (2.66) and neglecting terms of $O(1/N)$, we find

$$\begin{aligned} &\frac{1}{2} \sum_{k\mathrm{I}} A_k^2 \delta_k \cos(N + 1 - s)k \\ &\quad = \frac{1}{4} \sum_m [\cos(2 - \sigma)m\pi + \cos \sigma m\pi] A_{k_m}^2 \cos\left((1 - \sigma)\nu_m - \frac{m}{N}\right)\pi \qquad \text{(E-9)} \\ &\quad + \frac{1}{4} \sum_m [\sin(2 - \sigma)m\pi - \sin \sigma m\pi] A_{k_m}^2 \sin\left((1 - \sigma)\nu_m - \frac{m}{N}\right)\pi. \end{aligned}$$

The terms in brackets in each sum are rapidly oscillating functions of m while their coefficients are slowly changing functions of m, as $N \to \infty$. The sums are therefore $O(1/N)$ and can be neglected. Thus

$$G_{ij}^f = G_{i-j}^c, i \text{ odd} \quad \text{and} \quad j \text{ even}, \mid i - j \mid = o(N), i + j = O(N) \tag{E-10}$$

The same result holds for i even and j odd.

APPENDIX F. ALIGNMENT OF SPINS IN SUCCESSIVE IMPURITY PAIRS, HI MODEL

In this appendix we show that the spins of successive impurity pairs in the HI model are aligned parallel or antiparallel, depending on whether the number of elementary excitations (excluding the trivial $k = 0$ "excitation") is respectively odd or even. We shall consider only the special case that the impurity pairs are at opposite ends of a finite chain, but the generalization to any number of impurity pairs in any positions is obvious.

Although neither of the states Ψ_{0+} and Ψ_{0-} defined by (3.52d, e), are eigenstates of S_0^z or S_N^z, we wish to show that these two states involve only configurations

in which the first two spins are antiparallel to the last two. Because the first two spins (and also the last two) are themselves parallel, it is sufficient to show that

$$S^z{}_0 S^z{}_N \Psi_{0\pm} = -\tfrac{1}{4}\Psi_{0\pm} . \tag{F-1}$$

More generally, we shall show that

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} = -(-1)^n \tfrac{1}{4} \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \tag{F-2}$$

where $k_i \neq 0$ for all i.

Taking into account (3.41) and (3.43), we have

$$\begin{aligned} S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n} \Psi_{0\pm} &= -\tfrac{1}{4}(a_0{}^\dagger + a_0)(a_N{}^\dagger + a_N)\, \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= -\tfrac{1}{4} \exp(i\pi\mathfrak{N})(c_0{}^\dagger + c_0)(c_N{}^\dagger + c_N) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= -\tfrac{1}{4} \exp(i\pi\mathfrak{N})(\eta_0 \eta_0{}^\dagger - \eta_0{}^\dagger \eta_0) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= \pm\tfrac{1}{4} \exp(i\pi\mathfrak{N}) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \end{aligned} \tag{F-3}$$

where $\mathfrak{N} = \sum_0^N c_j{}^\dagger c_j$. Now it is easily seen that

$$\exp(i\pi\mathfrak{N}) \eta_k{}^\dagger \exp(-i\pi\mathfrak{N}) = -\eta_k{}^\dagger . \tag{F-4}$$

Therefore

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} = \pm\,(-1)^n \tfrac{1}{4} \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \exp(i\pi\mathfrak{N})\, \Psi_{0\pm} . \tag{F-5}$$

The result that the spin alignment of successive impurities goes from parallel to antiparallel or vice versa with each additional excitation is now obvious from the factor $(-1)^n$.

To determine the alignment in the states $\Psi_{0\pm}$ we must evaluate $\exp(i\pi\mathfrak{N})\Psi_{0\pm}$. First observe from (F-4) that

$$\eta_k \exp(i\pi\mathfrak{N})\Psi_{0-} = -\exp(i\pi\mathfrak{N})\eta_k \Psi_{0-} = 0, \quad \text{for all } k, \tag{F-6}$$

so that

$$\exp(i\pi\mathfrak{N})\Psi_{0-} = \exp(i\alpha)\Psi_{0-} , \tag{F-7}$$

where α is a phase angle to be determined. But

$$\exp(2i\pi\mathfrak{N}) = 1 \tag{F-8}$$

so that

$$\exp(i\alpha) = \pm 1. \tag{F-9}$$

from which we conclude that

$$\exp(i\pi\mathfrak{N})\Psi_{0\pm} = \pm\,\Psi_{0\pm} \tag{F-17}$$

and

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n}\Psi_{0\pm} = -(-1)^n \tfrac{1}{4}\eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n}\Psi_{0\pm}\,. \tag{F-18}$$

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Part XII

Delta Function Bose Gas

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Exact Analysis of an Interacting Bose Gas. I. The General Solution and the Ground State

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A gas of one-dimensional Bose particles interacting via a repulsive delta-function potential has been solved exactly. All the eigenfunctions can be found explicitly and the energies are given by the solutions of a transcendental equation. The problem has one nontrivial coupling constant, γ. When γ is small, Bogoliubov's perturbation theory is seen to be valid. In this paper, we explicitly calculate the ground-state energy as a function of γ and show that it is analytic for all γ, except $\gamma=0$. In Part II, we discuss the excitation spectrum and show that it is most convenient to regard it as a double spectrum—not one as is ordinarily supposed.

I. INTRODUCTION

IN comparatively recent times, as the history of quantum mechanics goes, a vast body of literature has developed on the quantum-mechanical problem of a gas or liquid of particles interacting via a two-body potential. To attack this problem, perturbation theory has been refined and developed in many elegant forms, too numerous and well known to attempt to summarize here. These results have been mainly of two kinds: attempts, based on summing series to all orders, to make exact statements about the true solution of the problem; and attempts to develop approximation schemes to yield quantitative results. It is fair to say, however, that few of these results may claim to be mathematically rigorous. They are accepted because they agree with our intuitive understanding of the problem.

Faced with such a situation it would seem desirable to find a local, time- and velocity-independent, two-body potential (the sort of potential that actually exists in a gas) such that, starting from the Schrödinger equation, and without introducing any approximations, one could derive the energy levels and wave functions of the system. It would also be desirable that such a model problem be three dimensional.

While there do exist several model many-body Hamiltonians in the literature, which are solvable, with one exception, none of them corresponds to having a simple potential of the character mentioned above. The one exception is the work of Girardeau[1] on a gas of impenetrable bosons in one dimension. He showed that the energy spectrum of such a gas is identical with the spectrum of a noninteracting Fermi gas. It is, indeed, unfortunate that, due to the inability of the particles to get past one another, Girardeau's model can only be thought of as an extreme high-density situation—even though the actual density of his gas may be low. By this is meant that if we attempt to draw a parallel between the one-dimensional hard-core model and the three-dimensional hard-core model, then the former resembles the latter only at very high densities when a cell model becomes applicable. In consequence of this fact, the model cannot be used to check any known form of perturbation theory.

Another drawback of Girardeau's model is that it is essentially a zero-parameter model. It might have been hoped that varying the density, ρ, or the hard-core radius, a, would modify the spectrum in some essential way, but this is not true. If $E_n(p)$ is any energy level of a state having momentum p, then $E_n(p)$ is of the form $[\rho/(1-\rho a)]^2 f_n([(1-\rho a)/\rho]p)$. In other words, the hard cores simply play the role of an excluded volume.

We shall propose here a model that in many respects is similar to Girardeau's, but which overcomes the two difficulties mentioned above. We consider a gas of bosons in one dimension interacting via a repulsive δ-function potential, whose Hamiltonian is given by Eq. (2.1) below. As we show, this problem has one nontrivial parameter, namely, $\gamma=\rho^{-1}c$, where $2c$ is the strength of the δ function. When $\gamma=\infty$ we obviously obtain Girardeau's results since the particles then are impenetrable. When $\gamma=0$ we have the noninteracting Bose gas.

A useful feature of this model is that for small γ Bogoliubov's perturbation theory[2] is valid. This is discussed in Sec. IV. The model agrees with all the predictions of that theory except in one important respect: For all values of γ the most convenient and natural way to view the spectrum of the gas is in terms of a double elementary boson excitation spectrum—not a single one as previous calculations have suggested. Bogoliubov's single spectrum agrees quite well with one of the spectra we obtain, but the other is totally unaccounted for in his theory. The principal value of this model perhaps lies in this startling fact. The whole question of the excitation spectrum, as well as some heuristic reason that this duplicity of the spectrum might have been anticipated, and why it might also exist in three dimensions, are discussed in the following paper.[3]

We may summarize the results of this paper as follows:

[1] M. Girardeau, J. Math. Phys. **1**, 516 (1960).

[2] See, for example, *The Many Body Problem*, edited by C. De Witt (John Wiley & Sons, Inc., New York, 1958), pp. 347–355.

[3] E. Lieb, following paper [Phys. Rev. **130**, 1616 (1963) (referred to here as II)].

With W. Liniger in Phys. Rev. *130*, 1605–1616 (1962)

(i) We obtain explicitly the eigenfunctions of the problem and show how they may be derived from the solution of a transcendental algebraic equation. This is the content of Sec. II.

(ii) In Sec. III we find the ground-state energy as a function of γ and show that in the limit of a large system it is analytic in γ except at $\gamma=0$. This shows that perturbation theory can at best hope to give an asymptotic series for the ground-state energy.

Most quantities of interest, such as the ground-state energy, the velocity of sound, the excitation spectra and others, derived both here and in II, have been calculated explicitly and numerical graphs are given. These quantities are derived from solutions to certain integral equations which cannot be found in closed form. The numerical work thus entailed was performed on an IBM 7090 computer. At the end of Appendix B, an outline of the numerical procedure is given. All of the properties of the solutions claimed above, however, such as their analyticity for $\gamma\neq 0$, have been rigorously proved.

II. THE PROBLEM AND THE NATURE OF ITS SOLUTIONS

We begin with the Schrödinger equation for N particles in one dimension interacting via a δ-function potential.[4]

$$(-\textstyle\sum_1^N(\partial^2/\partial x_i^2)+2c\sum_{\langle i,j\rangle}\delta(x_i-x_j))\psi=E\psi, \quad (2.1)$$

where $2c$ is the amplitude of the δ function. The region of space under consideration is

$$R: \quad \text{all } 0\leq x_i\leq L. \quad (2.2)$$

The wave function ψ satisfies periodic boundary conditions in each variable. We are interested in the repulsive case so that

$$c\geq 0. \quad (2.3)$$

While the attractive case, $c<0$, has a solution, it is not physically meaningful because there is no saturation. It is easy to demonstrate that in this case, for a fixed density, the ground-state energy is proportional to $-N^2$ instead of to $-N$.

It is well known that a δ-function potential is equivalent to the boundary condition

$$\left(\frac{\partial}{\partial x_j}-\frac{\partial}{\partial x_k}\right)\psi|_{x_j=x_k+}-\left(\frac{\partial}{\partial x_j}-\frac{\partial}{\partial x_k}\right)\psi|_{x_j=x_k-}$$
$$=2c\psi|_{x_j=x_k}; \quad (2.4)$$

i.e., ψ is continuous whenever two particles touch, but the jump in the derivative of ψ is $2c$. Moreover, since we are interested in symmetric (Bose) wave functions, the two terms on the left side of Eq. (2.4) are by definition equal.

[4] $\hbar=1$, $2m=1$. $\Sigma_{\langle i,j\rangle}$ means summation over pairs.

We can go one step further than this, however, and observe that if we define the region R_1 by

$$R_1: \quad 0\leq x_1\leq x_2\leq\cdots\leq x_N\leq L, \quad (2.5)$$

then knowledge of ψ in R_1 is equivalent to knowledge of ψ in R. Equations (2.1) and (2.4), thus, become

$$-\textstyle\sum_1^N(\partial^2/\partial x_i^2)\psi=E\psi \text{ inside} R_1, \quad (2.1a)$$

$$(\partial/\partial x_{j+1}-\partial/\partial x_j)\psi|_{x_{j+1}=x_j}=c\psi|_{x_{j+1}=x_j}. \quad (2.4a)$$

The original Schrödinger equation, (2.1) is thus replaced by a Helmholtz equation (2.1a) together with a mixed boundary condition (2.4a) on the boundary of R_1.

The last step is to interpret the periodic boundary conditions on R in terms of ψ defined in R_1. The periodic boundary condition reads in part

$$\psi(0,x_2,\cdots,x_N)=\psi(L,x_2,\cdots,x_N), \quad (2.6)$$

with a similar condition for the derivatives. The argument of the right-hand side of Eq. (2.6) is not in R_1, but by definition

$$\psi(L,x_2,\cdots,x_N)\equiv\psi(x_2,x_3,\cdots,x_N,L). \quad (2.7)$$

Hence, the original periodic condition is equivalent to the following boundary condition on R_1:

$$\psi(0,x_2,\cdots,x_N)=\psi(x_2,\cdots,x_N,L), \quad (2.8a)$$

$$\frac{\partial}{\partial x}\psi(x,x_2,\cdots,x_N)|_{x=0}=\frac{\partial}{\partial x}\psi(x_2,\cdots,x_N,x)|_{x=L}. \quad (2.8b)$$

Equations (2.8), together with Eq. (2.4a), now completely cover the entire boundary of R_1.

We now make the following *ansatz* for ψ: Let $\{k\}=k_1,\cdots,k_N$ be an ordered set of N numbers and define

$$\psi(x_1,\cdots,x_N)=\textstyle\sum_P a(P)P\exp(i\sum_{j=1}^N k_jx_j), \quad (2.9)$$

where the summation extends over all permutations of $\{k\}$, and $a(P)$ are certain coefficients depending on P. The wave function ψ is thus a generalization of the one-component Fermi function for which $a(P)$ would be $(-)^P$. It is to be understood that Eq. (2.9) defines ψ *only* in R_1, the extension to the rest of R following from the requirement of total symmetry under all particle permutations.

Can we choose $a(P)$ so that ψ satisfies the Schrödinger equation in R_1? Obviously Eq. (2.1a) is satisfied with

$$E=\textstyle\sum_1^N k_j^2. \quad (2.10)$$

Let us now examine Eq. (2.4a) when $x_1=x_2$. If all the k's are distinct (as will prove to be the case), then the $N!$ terms in Eq. (2.9) are linearly independent. Let P be the permutation that takes $\{k\}$ into $p, q, k_{\alpha_3},\cdots, k_{\alpha_n}$ and Q be the permutation that takes $\{k\}$ into $q, p, k_{\alpha_3},\cdots, k_{\alpha_n}$, where $q=k_{\alpha_1}$ and $p=k_{\alpha_2}$. If Eq. (2.4a) is to be satisfied, there must be a relationship between $a(P)$ and $a(Q)$ depending on p and q, and not involving the other $a(P)$'s. Denote by y the common value of x_1

and x_2 and substitute the two terms of ψ corresponding to P and Q into Eq. (2.4a). We must be able to satisfy

$$i(q-p)[a(P)-a(Q)]\exp(i(p+q)y+\textstyle\sum_{j=3}^{N} k_{\alpha_j}x_j) = c\exp(i(p+q)y+i\textstyle\sum_{j=3}^{N} k_{\alpha_j}x_j) \times[a(P)+a(Q)] \quad (2.11)$$

for all values of $y, x_3, \cdots, x_N$. This is, indeed, possible if

$$a(Q)=-a(P)\frac{c-i(q-p)}{c+i(q-p)}=-a(P)\exp(i\theta_{\alpha_1\alpha_2}), \quad (2.12)$$

where

$$\theta_{ij}=\theta(k_i-k_j), \quad (2.13a)$$

and

$$\theta(r)=-2\tan^{-1}(r/c). \quad (2.13b)$$

Assuming r to be real we have

$$\pi\geq\theta(r)\geq-\pi. \quad (2.13c)$$

Thus, by regarding ψ as the sum of $\frac{1}{2}(N!)$ pairs of terms corresponding to permutations such as P and Q above, we can satisfy Eq. (2.4a) for $x_1=x_2$ for each pair separately when the coefficients are given by Eq. (2.12).

The reader will easily verify that we can satisfy Eq. (2.4a) simultaneously for all $N-1$ possibilities $x_j=x_{j+1}$ if we choose the $a(P)$ in the following way: Let

$$a(I)=1. \quad (2.14)$$

Rule. If P takes $\{k\}$ into $\{k\}'=k_{\alpha_1}, \cdots, k_{\alpha_N}$, then rearrange $\{k\}'$ into $\{k\}$ by the process of transposing only adjacent k's. For each transposition, write down the factor $-e^{i\theta_{st}}$ where k_s and k_t are the transposed k's in question, k_s lying to the left of k_t before the transposition. The product of all such factors thus obtained is $a(P)$. There are, in general, many different ways to get $\{k\}'$ into $\{k\}$ but they all give rise to the same set of factors. For example, if

$$P=\begin{pmatrix}123\\321\end{pmatrix},$$

then for both the paths $(321)\rightarrow(231)\rightarrow(213)\rightarrow(123)$ and $(321)\rightarrow(312)\rightarrow(132)\rightarrow(123)$ we obtain the result $a(P)=-\exp i(\theta_{32}+\theta_{31}+\theta_{21})$.

An alternative definition of the above rule which makes it evident that $a(P)$ is indeed independent of the path is the following: Write down $k_1, \cdots, k_N$ in a line. Under it write down $k_{\alpha_1}, \cdots, k_{\alpha_N}$. For each k_j draw a straight line between the two points at which it occurs in the two rows. For each crossing point of two lines corresponding to k_α and k_β, $a(P)$ contains the factor $-e^{i\theta_{\alpha\beta}}$ where k_α precedes k_β in the set $\{k\}'$.

We conclude, therefore, that for *any* set $\{k\}$, ψ defined by Eq. (2.9) will satisfy Eqs. (2.1a) and (2.4a) when $a(P)$ is given by the above rule. There is one exception: All the k's in $\{k\}$ must be distinct, otherwise ψ will vanish identically. Condition (2.4a) determines only the form of ψ. The allowed values of the k's will be determined by Eq. (2.8). It is easily verified that these equations are equivalent to the N equations.

$$(-)^{N-1}e^{-ik_jL}=\exp(i\textstyle\sum_{s=1}^{N}\theta_{sj}), \quad \text{(all } j\text{)}, \quad (2.15)$$

where we have defined

$$\theta_{kk}=0. \quad (2.16)$$

Although Eqs. (2.15) are N equations in N unknowns, there will be many sets of solutions. The problem we have here is quite similar to the one-dimensional Heisenberg model of ferromagnetism with nearest neighbor interactions, first solved by Bethe.[5] Let us agree to order the k's (assuming they are real) so that

$$k_1<k_2<\cdots<k_N. \quad (2.17)$$

By observing that

$$\theta_{ij}=-\theta_{ji}, \quad (2.18)$$

and taking the product of all N equations in (2.15), we find that

$$\textstyle\sum_1^N k_j=2(\pi/L)n, \quad (2.19)$$

where n is an integer. We also find, by virtue of Eq. (2.13a), that if $\{k\}$ is a solution to Eq. (2.15), then the set $\{k'\}$ defined by

$$k_i'=k_i+2\pi n_0/L \quad (2.20)$$

is a solution for any integer n_0. The significance of Eq. (2.20) is the following: Since Eq. (2.9) defines ψ only in R_1, the k's cannot be regarded as true wave vectors. But the sum of the k's *is* a true wave vector and is, in fact, the total momentum of ψ; i.e.,

$$P_{\text{op}}\psi=(\sum_1^N(-i\partial/\partial x_j))\psi=(\sum_1^N k_j)\psi=p\psi \quad (\text{in}R). \quad (2.21a)$$

Equation (2.19) tells us that the total momentum must be an integral multiple of $2\pi/L$—an expected result. Equation (2.20) tells us that for any state with momentum p there is a state with momentum

$$p'=p+2\pi n_0\rho, \quad (2.21b)$$

where

$$\rho=N/L, \quad (2.22)$$

obtained by a simple shift of the k's. Conversely for any state with momentum $|p|\geq\pi\rho$ there is a corresponding state having a momentum in the range

$$-\pi\rho<p\leq\pi\rho. \quad (2.23)$$

We have, thus, to consider only states in the interval (2.23). All other states are obtained by the simple "umklapp," Eq. (2.20), which has the physical meaning of imparting a total momentum to the system while preserving the "internal" state of the system. The integer n_0 in Eq. (2.20) is thus one of the quantum numbers

[5] See R. Orbach, Phys. Rev. **112**, 309 (1958). This contains references to earlier papers.

describing a state. The energy of the new state is

$$E'=\sum_1^N (k_j')^2=E+\frac{4\pi n_0\rho}{N}p+\frac{1}{N}(2\pi n_0\rho)^2, \quad (2.24)$$

a well-known consequence of Galilean relativity.

To elucidate the nature of Eq. (2.15) we must study the two-body problem. To avoid loss of continuity we have relegated this to Appendix A. The principal results are as follows: (a) The *ansatz*, Eq. (2.9), appears to give all eigenstates of the problem; (b) for $\gamma>0$, the case in which we are interested, the k's are always real; (c) for $\gamma=0$ we obtain the noninteracting solution, while for $\gamma=\infty$ we obtain Girardeau's solution[6] with a continuous transition in between.

These same considerations apply to the N-particle case. Since the k's are real, we may order them according to Eq. (2.17). For real $\{k\}$ we can say something about the solution to Eq. (2.15). Dividing two successive equations and equating exponents, we have

$$\delta_j\equiv(k_{j+1}-k_j)L=\textstyle\sum_{s=1}^N(\theta_{s,j}-\theta_{s,j+1})+2\pi n_j \quad (j=1, 2, \cdots, N-1), \quad (2.25)$$

where n_j is an integer depending upon j, defined for $j=1, 2, \cdots, N-1$. These n_j's are the generalization of n_1 in Eq. (A3). Since θ_{kj} is a monotonically increasing function of j by Eqs. (2.13), the sum in Eq. (2.25) is negative. Therefore,

$$n_j\geq 1 \quad \text{(all } j\text{)}, \quad (2.26)$$

if there is to be a solution. Since

$$k_j=k_1+(1/L)\textstyle\sum_{s=1}^{j-1}\delta_s, \quad (2.27a)$$

and

$$k_\alpha-k_\beta=(1/L)\textstyle\sum_{s=\beta}^{\alpha-1}\delta_s \quad (\alpha>\beta), \quad (2.27b)$$

the right side of Eq. (2.25) involves only the δ's. Equation (2.25) is thus a self-contained set determining the δ's. If any set $\{n\}$ is chosen satisfying (2.26), there is presumably exactly one solution for the δ's. At least that was the case for two particles and will prove to be true for the cases we shall investigate involving a large number of particles. We also note that

$$\delta_j<2\pi n_j. \quad (2.28)$$

The remaining step is to determine the individual k's so as to satisfy Eqs. (2.15) and (2.23). If the $j=1$ equation of (2.15) is satisfied, the remainder will automatically be by virtue of Eq. (2.25). Thus, if we choose k_1 such that

$$k_1=-\frac{1}{L}\sum_{k=1}^N\theta_{k1}-\frac{2\pi m}{L}+\frac{\epsilon(N)}{L}$$

$$=-\frac{1}{L}\sum_{k=1}^N\theta\left(\frac{1}{L}\sum_{j=1}^{k-1}\delta_j\right)-\frac{2\pi m}{L}+\frac{\epsilon(N)}{L}, \quad (2.29)$$

where

$$\epsilon(N)=\pi \quad \text{for } N \text{ even}, \qquad =0 \quad \text{for } N \text{ odd}, \quad (2.30)$$

and m is some integer, and use Eq. (2.27a) to determine the other k's, Eq. (2.15) will be satisfied. To determine the integer m, which is not arbitrary, we observe that

$$p=\sum_1^N k_j=Nk_1+\frac{1}{L}\sum_{j=1}^{N-1}(N-j)\delta_j$$

$$=\frac{1}{L}\sum_{j=1}^{N-1}(N-j)\delta_j-\rho\sum_{j=1}^N\theta_{j1}-2\pi m\rho+\epsilon(N)\rho. \quad (2.31)$$

Equation (2.23) then fixes m.

As further support for the assertion that Eq. (2.25) has a unique solution for a given $\{n\}$, we shall consider the two limiting cases $c=0$ and $c=\infty$.

$c=\infty$: In this case all the θ's are zero, whence

$$\lim_{c\to\infty}\delta_j=2\pi n_j, \quad (2.32)$$

so that not only is the solution of (2.25) unique, but (2.28) becomes an equality. It is clear that we recover all Girardeau's wave functions and energies; the term $\epsilon(N)$ just gives the extra π mentioned in footnote 6 for the even N case.

$c=0$: By Eq. (2.13)

$$\lim_{c\to 0}\theta(x)=-\pi \quad \text{for } x>0 \qquad =\pi \quad \text{for } x<0, \quad (2.33)$$

and, hence, Eq. (2.25) yields

$$\lim_{c\to 0}\delta_j=2\pi(n_j-1). \quad (2.34)$$

There is, however, a *caveat*: if some $n_j=1$ then $\delta_j\to 0$, but it is then not clear that we can use the limiting form (2.33). We must ask for $\lim_{c\to 0}(\delta/c)$. Only if it is infinity can we use Eq. (2.33) and thereby obtain Eq. (2.34). But if $\delta\not\to 0$ Eq. (2.33) is certainly correct. Hence, by *reductio ad absurdum*, the only consistent conclusion is that Eq. (2.34) is always correct. The solution to Eq. (2.25) is again unique. We have, of course, recovered the well-known Bose functions for free particles. For N even, the $\epsilon(N)$ term in Eq. (2.31), which in this case is unwanted, is compensated by the term $\sum\theta_{j1}$.

We, thus, may conclude that the n_j are a complete set of "internal" quantum numbers for the system. Together with n_0 [Eq. (2.20)] they specify all states. By virtue of Eq. (2.28) moreover, the n_j may be thought of heuristically as the spacing between the k's.

[6] Girardeau obtained the solution to the hard-core problem only for N odd. For N even, however, there is an equally simple solution. One simply uses the Fermi function satisfying *antiperiodic* boundary conditions, i.e., $Lk=\pi+2n\pi$, where n is an integer. This exactly compensates the unwanted change of sign of his A function. For two particles the ground state has $k_2=-k_1=\pi/L$.

The exact spacing depends upon c to be sure, and also upon the relative position of δ_j in the set $\{\delta\}$. The fact that even for $n_j=$const the spacing is not uniform (except for $c=\infty$) gives rise to the principal difficulty in the analysis of the many-particle case. One other peculiarity of the problem should be remarked upon. The limiting case $c=\infty$ proved above to be particularly simple, but for $c\to 0$ the problem became pathological. Indeed, the latter limit will prove to be surprisingly delicate as we shall see.

III. GROUND-STATE ENERGY AND WAVE FUNCTION

We are interested in passing to the limit of a large system. This means N, $L\to\infty$ such that $\rho=$fixed constant. From dimensional considerations the ground-state energy can always be written

$$E_0=N\rho^2 l(N,cL), \tag{3.1}$$

where l is a dimensionless function of its arguments. But if E_0 is to be an extensive variable (as will, indeed, prove to be the case), l can depend only on intensive variables. The only dimensionless intensive variable in the problem is

$$\gamma=c/\rho. \tag{3.2}$$

Therefore,

$$E_0=N\rho^2 e(\gamma). \tag{3.3}$$

It is easy to show directly from Eq. (2.1) that $e(\gamma)$ is a monotonically increasing function of γ. We also expect that $e(0)=0$ (free particles) and $e(\infty)=\pi^2/3$ (Girardeau's solution). We can easily get an upper bound for $e(\gamma)$ by a variational calculation. Using the unperturbed Bose function, $\psi=1$, we obtain

$$e(\gamma)\leq\gamma. \tag{3.4}$$

Using Girardeau's function,[1] we have

$$e(\gamma)\leq\pi^2/3. \tag{3.5}$$

Returning to Eq. (2.25), it is clear that the choice

$$n_j=1 \tag{3.6}$$

gives the ground state, for this choice minimizes the δ's and hence allows the k's to be as close to zero as possible. We also see from the symmetry of the equations that if k is in $\{k\}$, then so is $-k$. Indeed this is always so for $n_j=$const and implies that $p=0$ for such states. Equation (2.31) determines k_1 in this case:

$$-k_1=\frac{1}{NL}\sum_1^{N-1}(N-j)\delta_j=k_N\equiv K(\gamma). \tag{3.7}$$

From Eq. (2.28) *et seq.* we see that

$$K(0)=0,\quad K(\infty)=\pi\rho, \tag{3.8}$$

with presumably a continuous monotonic transition in between.

We are, thus, led to expect that $K(\gamma)$ is an intensive variable and that the process of passing to an infinite system consists in "filling in" more and more points in the set $\{k\}$ between $-K$ and K with the understanding that the spacing between k's may not be uniform. This may be shown as follows: The inequality $k_{j+1}-k_j<2\pi/L$, Eq. (2.28), permits us for a large system to use a Taylor expansion in Eq. (2.25), i.e.,

$$\theta(k_s-k_j)-\theta(k_s-k_{j+1})=-2c(k_{j+1}-k_j)\frac{1}{c^2+(k_s-k_j)^2}+O(1/L^2), \tag{3.9}$$

and, hence,

$$(k_{j+1}-k_j)=-2c(k_{j+1}-k_j)\frac{1}{L}\sum_{s=1}^{N}[c^2+(k_s-k_j)^2]^{-1}+\frac{2\pi}{L}+O(1/L^2). \tag{3.10}$$

Define

$$k_{j+1}-k_j=1/Lf(k_j), \tag{3.11}$$

by means of which the sum in Eq. (3.10) may be approximated by an integral by Poisson's formula to the required accuracy in L^{-1}. Equation (3.10) becomes

$$2c\int_{-K}^{K}\frac{f(p)}{c^2+(p-k)^2}dp=2\pi f(k)-1. \tag{3.12}$$

The meaning of $f(k)$ is that for a large system

$$Lf(k)dk=\text{number of } k\text{'s in } (k,\ k+dk). \tag{3.13}$$

The subsidiary condition determining the number of particles is

$$\int_{-K}^{K}f(k)dk=\rho, \tag{3.14}$$

while the ground-state energy is given by

$$E_0=\sum_1^N k_j^2=\frac{N}{\rho}\int_{-K}^{K}f(k)k^2dk. \tag{3.15}$$

One final condition implied by Eqs. (3.11) and (3.13) is

$$f(k)\geq 0. \tag{3.16}$$

Let us change variables as follows: Define

$$k\equiv Kx;\quad c\equiv K\lambda;\quad f(Kx)\equiv g(x), \tag{3.17}$$

in terms of which Eqs. (3.12), (3.14), and (3.15) become, respectively,

$$1+2\lambda\int_{-1}^{1}\frac{g(x)dx}{\lambda^2+(x-y)^2}=2\pi g(y), \tag{3.18}$$

$$e(\gamma)=\frac{\gamma^3}{\lambda^3}\int_{-1}^{1}g(x)x^2dx, \tag{3.19}$$

$$\gamma\int_{-1}^{1}g(x)dx=\lambda. \tag{3.20}$$

The program, therefore, consists of the following steps: (i) Solve Eq. (3.18) for a fixed λ; (ii) use Eq. (3.20) to determine λ as a function of γ; (iii) Eq. (3.19) then gives $e(\gamma)$; (iv) Eq. (3.17) gives $K(\gamma)$, i.e.,

$$K=\rho\gamma\lambda^{-1}=\rho\left[\int_{-1}^{1}g(x)dx\right]^{-1}. \tag{3.21}$$

Equation (3.18) is an inhomogeneous Fredholm equation of the second kind with an inhomogeneous term that is positive definite (i.e., $+1$). In Appendix B we discuss this equation in considerable detail and prove the following:

(a) For *any* inhomogeneous term there is exactly one solution $g(y)$.

(b) $g(y)$ is an infinitely differentiable (analytic) function of λ for $\lambda>0$.

(c) If the inhomogeneous term is positive definite [as in Eq. (3.18)], $g(y)>0$ for all y.

(d) If the inhomogeneous term is bounded above (below), then $g(y)$ is bounded above (below).

These statements enable us to claim that $g(y,\gamma)$, $e(\gamma)$, and $K(\gamma)$ are analytic functions of γ (except for $\gamma=0$). Since there are then no unusual kinks or points of discontinuous derivatives, it becomes a straightforward matter to evaluate all quantities numerically with confidence. The proof is as follows: (b) and (c) above, together within Eq. (3.20), imply that γ is an analytic function of λ for λ in $(0,\infty)$. Equation (3.19) then implies that e is analytic in λ; Eq. (3.21) implies that K is analytic in λ. The problem is then to prove that (i) λ is an analytic function of γ and that (ii) the range $0<\lambda<\infty$, in fact, covers the required range $0<\gamma<\infty$. By the implicit function theorem, statement (i) will be true if we can show that

$$0\neq\frac{\partial\gamma}{\partial\lambda}=\left[\int_{-1}^{1}g(x)dx\right]^{-2}$$
$$\times\left\{\int_{-1}^{1}g(x)dx-\lambda\int_{-1}^{1}\frac{\partial}{\partial\lambda}g(x)dx\right\}, \tag{3.22}$$

for all λ. By (b) above, $[\int_{-1}^{1}g(x)dx]^{-2}\neq0$. As for the two terms in { }, we observe that if we define

$$h(x,\lambda)\equiv\left(\frac{\partial}{\partial\lambda}+\frac{x}{\lambda}\frac{\partial}{\partial x}\right)g(x,\lambda), \tag{3.23}$$

and integrate Eq. (3.18) by parts several times, we easily obtain an equation for h, viz.,

$$2\pi h(y,\lambda)=2\lambda\int_{-1}^{1}dx\frac{h(x,\lambda)}{\lambda^2+(x-y)^2}$$
$$-2g(1,\lambda)\left(\frac{1}{\lambda^2+(y+1)^2}+\frac{1}{\lambda^2+(y-1)^2}\right). \tag{3.24}$$

By (c) above, the inhomogeneous term in Eq. (3.24) is negative definite and, consequently, $h(x,\lambda)<0$ [by then applying (c) to Eq. (3.24)]. We have, therefore,

$$0>\lambda\int_{-1}^{1}h(x,\lambda)dx$$
$$=\int_{-1}^{1}\left(\lambda\frac{\partial g(x,\lambda)}{\partial\lambda}-g(x,\lambda)\right)dx+2g(1,\lambda) \tag{3.25}$$

by using the definition (3.23) and integrating by parts. Since $g(1,\lambda)>0$, the integral in Eq. (3.25) is negative definite. But this integral is just the negative of the term in { } in (3.22). Hence, statement (i) above is proved. We see, incidently, that λ and γ are monotonically increasing functions of each other.

As for (ii) above, we see from Eq. (3.18) that

$$\lim_{\lambda\to\infty}g(x,\lambda)=1/2\pi, \tag{3.26}$$

and, consequently, from Eq. (3.20)

$$\lim_{\lambda\to\infty}\gamma=\infty. \tag{3.27a}$$

As $\lambda\to0$, on the other hand, the bounds mentioned in (d) above guarantee that $g(x,\lambda)\not\to0$. [On the contrary $g(x,\lambda)\to\infty$ in this limit.] Equation (3.20) then implies that

$$\lim_{\lambda\to0}\gamma=0. \tag{3.27b}$$

Equations (3.27) establish (ii) above.

To recapitulate, we have shown that all quantities are analytic functions of γ in $(0,\infty)$. As the above arguments tend to suggest, however, and as we, in fact, show later, there is a very serious singularity at $\gamma=0$. The physical meaning of this singularity is that any interaction, however weak (but volume-independent), leads in the limit of a large system to a system that is in some way basically different from the noninteracting case. If one tries to find a series for $e(\gamma)$ for small γ, such a series can at best be asymptotic—a result already indi-

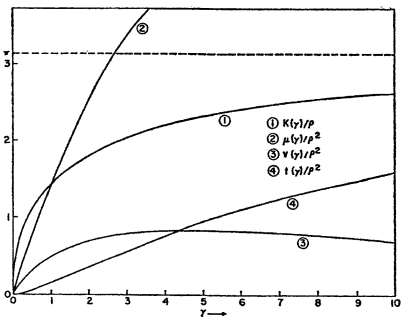

FIG. 1. Various numerically derived properties of the ground state plotted as functions of $\gamma=c/\rho$. K=cutoff momentum, μ=chemical potential, v=potential energy per particle, and t=kinetic energy per particle. As $\gamma\to\infty$: $K\to\pi\rho$; $\mu\to\pi^2\rho^2$, $v\to0$, and $t\to\frac{1}{3}\pi^2\rho^2$.

cated, but not proved, by the conventional perturbation theoretic treatments.

In Appendix B an outline is given of the numerical solution of Eqs. (3.18–20). While nonpathologic behavior is guaranteed by the above analyticity considerations, the singularity at $\gamma=0$ makes the numerical calculation more and more difficult as this limit is approached.

In plotting results we use units in which $\rho=1$, so that K/ρ varies between 0 and π. We have also eliminated the dependent parameter λ in favor of the independent parameter γ by using Eq. (3.20). [Numerical values of λ as a function of γ can be obtained, if desired, from the relation $\lambda=\gamma(K/\rho)^{-1}$, Eq. (3.21).] Figure 1

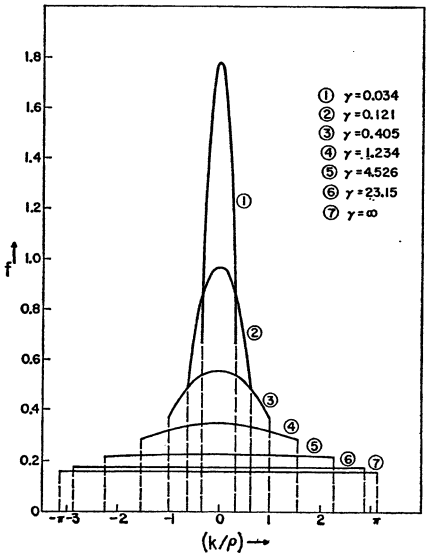

FIG. 2. The distribution function of "quasi-momenta" in the ground state for various values of $\gamma=c/\rho$. The vertical dashed lines are the cutoff momenta K (cf. Fig. 1). When $\gamma=\infty$, $f=(2\pi)^{-1}$. For all γ, $\int_{-K}^{K} f(k)dk=\rho$.

shows $K(\gamma)$ while Fig. 2 shows the density function $f(k,\gamma)$ for several values of γ. It will be noticed that as $\gamma\to 0$ small values of k become relatively more important. Figure 3 shows the end result of the calculation, $e(\gamma)$. The straight dashed line is the zeroth-order perturbation theory result $e=\gamma$, which also coincides with the primitive upper bound obtained before [Eq. (3.4)]. The other dashed curve, $e=\gamma[1-(4/3\pi)\sqrt{\gamma}]$, is the result of Bogoliubov's perturbation theory which we shall discuss presently. It is in fair agreement with the exact answer up to $\gamma=2$. We may, therefore, regard $0\leq\gamma<2$ as the weak coupling region. On the other hand, it is interesting to note that even for $\gamma=10$, $e(\gamma)$ is

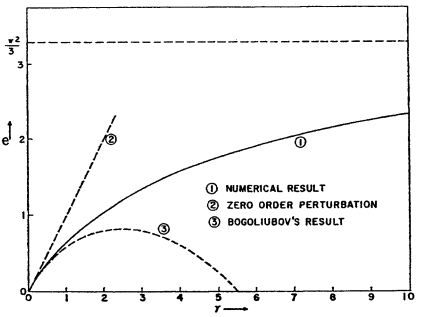

FIG. 3. The ground-state energy $E_0=N\rho^2 e(\gamma)$. The full curve gives $e(\gamma)$ obtained numerically. As $\gamma\to\infty$, $e\to\frac{1}{3}\pi^2$. Curve 2 is the zero-order perturbation theory result, i.e., the expectation value of the potential in the noninteracting ground state. Curve 3 is the result of Bogoliubov's perturbation theory, which is seen to be good up to $\gamma\sim 2$.

still quite far from its asymptotic limit, $\frac{1}{3}\pi^2$. In fact, in order to get within 10% of this asymptotic limit γ must be about 37. The intermediate coupling region, by one definition at least, is, therefore, $2<\gamma<37$.

There are other quantities of interest in connection with the ground state; these are also plotted in Fig. 1. There is the chemical potential μ, or energy necessary to add one particle to the system, defined by

$$\mu=\frac{\partial E_0}{\partial N}=\rho^2\left(3e-\gamma\frac{de}{d\gamma}\right). \tag{3.28}$$

Also interesting is the potential energy per particle v, which by a well-known theorem is

$$v=\frac{c}{N}\frac{\partial}{\partial c}E_0=\rho^2\gamma\frac{de}{d\gamma}, \tag{3.29}$$

and the kinetic energy per particle

$$t=\frac{1}{N}E_0-v=\rho^2\left(e-\gamma\frac{de}{d\gamma}\right). \tag{3.30}$$

We conclude this section with a list of the asymptotic forms of the various quantities for large and small γ.

Large γ. This is the easiest case. The denominator in the integral of Eq. (3.18) may be effectively replaced by λ^2. The error thus introduced in the integral is small, but by Eq. (3.26) the integral itself is small compared to 1, so that the resultant error in g will be quite small indeed. This substitution leads to $g(x)=\text{const}$ which may be readily evaluated as

$$g(x)=\lambda(2\pi\lambda-4)^{-1}. \tag{3.31}$$

Substitution of Eq. (3.31) into Eqs. (3.19) and (3.20)

leads (for large γ) to

$$\lambda=\frac{1}{\pi}-(\gamma+2), \quad e=\tfrac{1}{3}\pi^2\left(\frac{\gamma}{\gamma+2}\right)^2, \quad K=\pi\frac{\gamma}{\gamma+2}\rho,$$
$$\mu=\frac{3\gamma+2}{\gamma+2}\rho^2 e, \quad v=\frac{4}{\gamma+2}\rho^2 e, \quad t=\frac{\gamma-2}{\gamma+2}\rho^2 e. \tag{3.32}$$

These results are accurate to 1% for γ as small as 10.

Small γ. As we show in Appendix B, as $\lambda\to 0$ the factor 2π on the right side of Eq. (3.18) becomes an eigenvalue of the integral equation. Consequently, $g(x,\lambda)$ has a singularity at $\lambda=0$. In addition to this difficulty, the kernel of the integral equation also becomes quite pathological. It will be recognized that as $\lambda\to 0$ the kernel becomes a well-known representation for $2\pi\delta(x-y)$ so that in this limit Eq. (3.18) reads: $2\pi g(x)=2\pi g(x)+1$. It is clear, therefore, that in this limit g becomes unbounded—a statement borne out by the limits on g given in Appendix B.

There does not seem to be any simple way to get a systematic, reliable expansion of g as $\lambda\to 0$. We can, however, guess the zeroth order form for g:

$$g(x,\lambda)\sim\frac{1}{2\pi\lambda}(1-x^2)^{1/2}, \quad (\lambda\to 0) \tag{3.33}$$

and one can then show, using bounding arguments similar to those in Appendix B, that the correction to (3.33) is of higher order in λ for all x, and is positive definite. Beyond this, we have been unable to obtain an unambiguous correction to (3.33). One of the major difficulties is deciding what happens at the end points, $|x|=1$.

Equation (3.33) allows us to find only the leading term for the quantities mentioned in (3.32). These turn out to be (for small γ)

$$\lambda=\tfrac{1}{2}\sqrt{\gamma}, \quad e=\gamma, \quad K=2\rho\sqrt{\gamma},$$
$$\mu=2\rho^2\gamma, \quad v=\gamma, \quad t=0. \tag{3.34}$$

The equation $e=\gamma$ is plotted in Fig. 3. We see that the upper bound for e [Eq. (3.4)] is, in fact, its asymptotic form—a result predicted by elementary perturbation theory.

It will be noticed from Fig. 1, as well as from Eqs. (3.32) and (3.34) ,that for small γ the potential energy dominates the kinetic. The reverse is true for large γ; in fact $v\to 0$ as $\gamma\to\infty$. This behavior is exactly the same as for three dimensions—it is often said that a large potential behaves like a kinetic energy barrier. This fact is supposed by some to be tied up with the ability of particles to "go around" each other in three dimensions. But as we can clearly see, it is also present in one dimension. Thus, the difference between one and three dimensions does not lie here—it is apparently immaterial to the particles whether they can "get around" each other or merely "through" each other.

IV. PERTURBATION THEORY

The well-known perturbation theory of Bogoliubov[2] was at first assumed to be an expansion in the density. That this is incorrect was realized when it was found that the correct parameter for a low-density expansion is the scattering length (in three dimensions) and not $\int v(x)d^3x$ as appears in Bogoliubov's theory. But Bogoliubov's theory *is* asymptotically correct if we regard it as an expansion in the potential. In other words, it may be expected to give the first two terms in the energy correctly for any density if the potential is so weak that it may be treated by the Born approximation. In our case, therefore, the Bogoliubov theory should be correct for small γ. On the other hand, small γ may be thought of as high density—the reverse of the usual (incorrect) assumption mentioned above.

This last observation leads to a second reason for believing in the Bogoliubov result for small γ. One can show (we shall not do so here) that if the Fourier transform of the potential is everywhere nonnegative, then Bogoliubov's theory is correct—at least as far as the ground-state energy is concerned—in the limit of *high* density. The δ-function potential certainly satisfies the above criterion.

As stated in the introduction, one of the uses of an exact model is as a check for approximation schemes. It is indeed fortunate that the present model has a definite range of coupling constant over which the Bogoliubov theory may be unambiguously expected to be correct. Our model, therefore, should serve not only to establish the validity of the Bogoliubov theory but should also serve as an indicator (taking appropriate account of the difference between one and three dimensions) of the range over which the theory is reasonably accurate.

The Bogoliubov prescription easily yields the following results: The spectrum of elementary excitations is given by

$$\epsilon(p)=\rho^2|p/\rho|[(p/\rho)^2+4\gamma]^{1/2}. \tag{4.1}$$

We have purposely written $\epsilon(p)$ in terms of the dimensionless variable p/ρ. The ground-state energy is given by

$$E_0=\tfrac{1}{2}N^2(2c/L)+\tfrac{1}{2}\sum_p[\epsilon(p)-p^2-N(2c/V)]$$
$$=N\rho^2\gamma[1-(4/3\pi)\sqrt{\gamma}]. \tag{4.2}$$

The expression for $e(\gamma)$, (4.2) is plotted in Fig. 3; it is adequate up to approximately $\gamma=2$. Equation (3.34) shows the leading term is exact. While we have not found an analytic expression for the second term, $(4/3\pi)\gamma^{3/2}$, the numerical results of Fig. 3 indicate that it too is correct. It is interesting to note that the exact equation for $e(\gamma)$ is so pathological at $\gamma=0$ that it was an effort to find even the zeroth-order term for $e(\gamma)$, while perturbation theory gives the first two terms by elementary quadrature.

As for the elementary excitations, we shall show in II that Eq. (4.1) is also fairly accurate up to about $\gamma=2$, but that there is another type of elementary excitation unaccounted for by Bogoliubov's theory.

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APPENDIX A. THE TWO-BODY PROBLEM

To elucidate the nature of Eqs. (2.15), we shall study the two-body problem. To highlight the basic difference between the repulsive and attractive cases, we shall consider both. For the two-body problem, (2.15) becomes

$$-e^{ik_2L}=e^{i\theta_{21}}=-e^{-ik_1L}. \tag{A1}$$

There are several ways to solve this problem and we shall choose one which may be generalized to the N-body case. Define

$$(k_2-k_1)L=\delta, \quad \gamma=\tfrac{1}{2}cL, \tag{A2}$$

then, multiplying the two equations (A1), we obtain

$$\begin{aligned}\delta&=2\theta(k_2-k_1)+2\pi n_1 \\ &=-4\tan^{-1}(\delta/2\gamma)+2\pi n_1,\end{aligned} \tag{A3}$$

where n_1 is an integer. If we invert Eq. (A3) we obtain

$$\delta/2\gamma=-\tan(\delta/4), \quad n_1 \text{ even} \tag{A4a}$$

$$=[\tan(\delta/4)]^{-1}, \quad n_1 \text{ odd}. \tag{A4b}$$

It must be remembered that Eqs. (A4) have far more solutions than Eq. (A3) (because $|\theta|<\pi$ by definition). Now if $z\tan z=$ real, then z is either real or imaginary, not complex. The same applies if $(1/z)\tan z=$ real. Hence, the roots of Eq. (A3) are either real or imaginary. For the real roots we choose δ positive in accordance with (2.17). For $\gamma>0$ (repulsive case), there are, in fact, only real roots as Eqs. (A4) show. For every solution to either Eq. (A4a) or (A4b) there exists an integer n_1 such that Eq. (A3) is satisfied, and conversely for every integer $n_1\geq 1$ there is a unique positive solution to Eq. (A3) given by either (A4a) or (A4b). The single exception is $n_1=0$ for which there can be no solution because the first term on the left side of Eq. (A3) is negative ($\delta=0$ is not allowed). We see that

$$2\pi(n_1-1)<\delta<2\pi n_1. \tag{A5}$$

In the limiting cases the roots corresponding to $n_1=1$, 2, 3, etc., are, respectively,

$$\delta=0,\ 2\pi,\ 4\pi, \text{ etc.} \quad (\gamma=0) \tag{A6a}$$

$$\delta=2\pi,\ 4\pi,\ 6\pi, \text{ etc.} \quad (\gamma=\infty). \tag{A6b}$$

We have now to determine k_1 and k_2 separately so as to satisfy Eqs. (A1). Substituting the value of θ_{21} from Eq. (A3) into Eq. (A1) we see that for every root, δ, there is in fact a unique solution satisfying (2.23) given by

$$Lk_2=-Lk_1=\tfrac{1}{2}\delta; \quad p=0, \quad (n_1 \text{ odd}) \tag{A7a}$$

$$Lk_2=\tfrac{1}{2}\delta+\pi; \quad Lk_1=-\tfrac{1}{2}\delta+\pi;$$
$$p=2\pi/L=\pi\rho, \quad (n_1 \text{ even}). \tag{A7b}$$

Thus, we see that for every integral value of $n_1\geq 1$ there corresponds a unique state having a definite energy and a momentum in the range (2.23). The integer n_1 may, therefore, be considered the second or "internal," quantum number of the problem which, together with n_0, specifies a state. The ground state corresponds to $n_1=1$ and has zero momentum as expected.

For $\gamma<0$ (attractive case), the situation is more complicated and rather surprising. The real roots are much the same as before except that here $n_1=0$ becomes permissible if $\gamma>-2$. Equation (A5) is changed to

$$2\pi n_1<\delta<2\pi(n_1+1), \tag{A5a}$$

while Eqs. (A7) remain unaltered. For the imaginary roots, it is wise to return to the original definition of $e^{i\theta}$ [Eq. (2.12)] in order to avoid ambiguity in the definition of $\tan^{-1}$. One finds that for $n_1=1$ there is always a pair of equal and opposite imaginary roots given by Eq. (A4b). Only one of them need be considered, for the other corresponds to interchanging k_1 and k_2. If we write $\delta=i\alpha$ ($\alpha>0$), then

$$\alpha>-2\gamma. \tag{A8}$$

By Eq. (A7a) this state has zero momentum and its energy is

$$E_0=-(1/2L^2)\alpha^2<-\tfrac{1}{2}c^2. \tag{A9}$$

This state, which is the ground state of the problem, is the analog of the single bound state for an attractive delta function in infinite space for which $E_0=-\frac{1}{2}c^2$, $\psi=\exp(-\frac{1}{2}c|x_1-x_2|)$. Putting the particles in a box with infinite walls (zero boundary conditions) would reduce the binding energy, however, contrary to Eq. (A9). The periodic boundary conditions are responsible for this anomalous result.

Even more surprising is the appearance of a second bound state. We saw above that for $\gamma>-2$ there is an $n_1=0$ real solution. In this case there is no other bound state. But if $\gamma<-2$ (strong coupling) the real solution for $n_1=0$ disappears in favor of an imaginary solution

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to Eq. (A4a). For this solution

$$\alpha' < -2\gamma. \tag{A10}$$

By Eq. (A7b) this state has a momentum $p=2\pi/L$ and an energy

$$E_0' = -\frac{1}{2L^2}(\alpha')^2 + \frac{2}{L^2}\pi^2 > -\tfrac{1}{2}c^2. \tag{A11}$$

For $\gamma=-2$ the $n_1=0$ root is $\delta=0$ which must be discarded. On the other hand, the state cannot disappear for a single value of γ. The paradox is resolved by taking the limit $\gamma \to -2$, whereupon we find

$$\psi' = [2+c(x_2-x_1)] \exp\left[i\frac{\pi}{L}(x_1+x_2)\right], \quad (\gamma=-2), \tag{A12}$$

in R_1. Two facts should be noticed about this second bound state. Firstly, it has a nonzero momentum, but it does *not* correspond to the translation of a bound state with $p=0$. Translated states of two particles with zero momentum must have momenta which are integral multiples of $4\pi/L$. Secondly, this state does not disappear in the limit $L \to \infty$ as might have been hoped. In fact, for *any* fixed c we can always choose L large enough such that $\gamma < -2$ and this second state will make its appearance. As $L \to \infty$ both inequalities (A8) and (A10) approach equalities so that E_0 and E_0' becomes asymptotically degenerate and equal to the infinite space binding energy.

Having obtained these wave functions we may ask if the *ansatz* Eq. (2.9) [with the single exception, Eq. (A12)] exhausts all the solutions of the Schrödinger equation. It seems clear that it, in fact, does so, at least for the repulsive case, although we cannot prove that this is true. We are led to this view because in the repulsive case we obtain the well-known wave functions for $\gamma=0$ (free particles) and we obtain Girardeau's solution for $\gamma=\infty$ (hard cores), with a continuous transition from one to the other. For $\gamma<0$, on the other hand, the situation is not quite so clear. As $\gamma \to 0$ we recover the free particle solutions. For $\gamma \neq 0$ we can only observe that as $L \to \infty$ we obtain the well-known bound state and scattering solutions for the attractive δ-function potential.

These same considerations apply to the N-particle problem and we shall therefore suppose that Eqs. (2.9) and (2.15) yield all the wave functions of the problem for the repulsive case.

From consideration of the two-body problem we are led to the following hypothesis: For the repulsive case every solution $\{k\}$ contains only real k's, which we may, therefore, order according to (2.17). For the attractive case, which we shall not consider further, complex k's may appear. One should expect many types of nonreal solutions for $\gamma<0$ corresponding to two-body, three-body, etc., bound states.

APPENDIX B. SOLUTION OF THE BASIC INTEGRAL EQUATION

I. Existence, Uniqueness, and Analyticity of the Solution

(i) The integral equation (3.18) is a special case of

$$r(y) + \int_{-1}^{1} K(y-x)g(x)dx = \sigma g(y), \tag{B1}$$

where

$$K(y) = 2\lambda/(\lambda^2+y^2)$$

and $\lambda>0$. Equation (B1) can be brought into the form

$$u(s) - \mu\int_{-a}^{a} R(s-t)u(t)dt = v(s), \tag{B2}$$

by letting $y=\lambda s$, $x=\lambda t$, $a=1/\lambda<\infty$, $\mu=2/\sigma$, $u(s)=g(y)$, $v(s)=r(y)/\sigma$, and

$$R(s,t) = R(s-t) = 1/[1+(s-t)^2]. \tag{B3}$$

By definition,[7] R is positive definite if

$$J_a = \int_{-a}^{a}\int_{-a}^{a} R(s,t)u(s)u(t)dsdt > 0, \tag{B4}$$

for any square integrable $u(s) \not\equiv 0$. For R to be positive definite with respect to the interval $(-a, a)$ it is sufficient that R be positive definite with respect to $(-\infty, \infty)$ because the square integrable functions with respect to $(-a, a)$ can be thought of as a subset of square integrable functions with respect to $(-\infty, \infty)$ which vanish identically for $|s|>a$. Let

$$\eta(s) = \int_{-\infty}^{\infty} R(s-t)u(t)dt \quad \text{and} \quad u^*(p), \eta^*(p)$$

be the Fourier transforms of $u(s)$ and $\eta(s)$, respectively. Then, according to Parseval's equation,[8] and because $\eta(s)$ is real,

$$J_\infty = \int_{-\infty}^{\infty} u(s)\eta(s)ds = \int_{-\infty}^{\infty} u^*(p)\bar{\eta}^*(p)dp.$$

As $\eta(s)$ is defined by a convolution, one has

$$\eta^*(s) = (2\pi)^{1/2}R^*(p)u^*(p),$$

and, thus

$$J_\infty = (2\pi)^{1/2}\int_{-\infty}^{\infty} \bar{R}^*(p)|u^*(p)|^2 dp.$$

[7] R. Courant and D. Hilbert, *Methoden der Mathematischen Physik* (Springer-Verlag, Berlin, 1931), Vol. I, p. 105.

[8] W. Schmeidler, *Integralgleichungen mit Anwendungen in Physik und Technik* (Akademische Verlagsgesellschaft, Leipzig, 1955), Vol. 1, pp. 74, 75.

It is well known[9] that

$$R^*(p)=\bar{R}^*(p)=(\pi/2)^{1/2}e^{-|p|}>0,$$

and, thus, $J_\infty>0$ except for $u(s)\equiv 0$, that is (B4) is proved. Since R is positive definite, all eigenvalues of (B1) or (B2) are positive.[10]

(ii) Consider the kernel R and its iterates[11]

$$R^{(1)}(s,t)=R(s,t), \tag{B5a}$$

$$R^{(i+1)}(s,t)=\int_{-a}^{a}R^{(i)}(s,\tau)R(\tau,t)d\tau, \quad (i\geqq 1). \tag{B5b}$$

From the defintion (B3) of R it is evident that there exist constants $C_j>0$ such that $|\partial^j R^{(1)}/\partial s^j|\leqq C_j$ for any $j\geqq 0$. One has

$$\int_{-a}^{a}R(\tau,t)d\tau=T(a,t)=\arctan(a-t)+\arctan(a+t). \tag{B6}$$

It is easy to see that

$$\pi/2<\arctan 2a\leqq T(a,t)\leqq 2\arctan a=\pi-\epsilon, \quad \epsilon>0. \tag{B7}$$

Assume now that, for a certain $i\geqq 1$ and any $j\geqq 0$,

$$|\partial^j R^{(i)}(s,t)/\partial s^j|\leqq C_j(\pi-\epsilon)^{i-1}.$$

Then, because $\partial^j R^{(i)}(s,t)/\partial s^j$ is continuous in s for all j, one can differentiate under the integral sign and, using (B7), one gets

$$\left|\frac{\partial^j R^{(i+1)}(s,t)}{\partial s^j}\right|=\left|\int_{-a}^{a}\frac{\partial^j R^{(i)}(s,\tau)}{\partial s^j}\times R(\tau,t)d\tau\right|\leqq C_j(\pi-\epsilon)^i. \tag{B8}$$

As (B8) holds for $i=0$ it follows by induction that (B8) holds for all $i\geqq 0$. Therefore, the Neumann series and its derivatives with respect to s taken term by term, that is,

$$\frac{\partial^j\rho(s,t)}{\partial s^j}=\sum_{i=0}^{\infty}\mu^i\frac{\partial^j R^{(i+1)}(s,t)}{\partial s^j} \tag{B9}$$

for $j\geqq 0$, converge absolutely and uniformly in both variables s and t for all $\mu<1/(\pi-\epsilon)$. The same result holds for the derivatives with respect to t as can be proved in a similar way.

From the uniform convergence of the Neumann series for $j=0$ follows first the existence of the resolvent kernel, $\rho(s,t)$, in particular for $\mu=1/\pi$, and the validity of the representation[12]

$$u(s)=v(s)+\mu\int_{-a}^{a}\rho(s,t)v(t)dt, \tag{B10}$$

or of the equivalent representation

$$g(y)=\frac{1}{\sigma}r(y)+\frac{1}{\sigma^2}\int_{-1}^{1}\kappa(y,x)r(x)dx, \tag{B11a}$$

$$\kappa(y,x)=\sum_{i=0}^{\infty}\sigma^{-i}K^{(i+1)}(y,x). \tag{B11b}$$

The eigenvalues of (B2) are, thus, all $\geqq 1/(\pi-\epsilon)$ and those of (B1) are $\leqq 2\pi-2\epsilon$. Property (a) of Sec. III, that is, the existence of a unique solution of Eq. (B1) for $\sigma=2\pi$, is thus proved. From the uniform convergence of the series in (B9) with $j\geqq 1$ follows the analyticity of the resolvent kernel with respect to s and t.

(iii) Let $\lambda=z$ be complex in the expressions for the kernel K and its iterates. Consider a closed circular domain $\bar{D}$ defined by $|z-\lambda_1|\leqq\delta$, with real λ_1, δ and $0<\delta<\lambda_1/\sqrt{2}$. Then, if y is real, it is easy to see that $|K(y;z)|\leqq 2(\lambda_1+\delta)/(\lambda_1-\delta)^2$ for any $z\epsilon\bar{D}$. Let $[\pi-\epsilon_1(\delta)]=2\arctan[2/(\lambda_1-\delta)]$, $\epsilon_1(\delta)>0$. As $\delta\to 0$, the quantity $q(\delta)=[(\lambda_1+\delta)/(\lambda_1-\delta)]$. $[\pi-\epsilon_1(\delta)]$ decreases monotonically to $(\pi-\epsilon)=2\arctan(2/\lambda_1)$, where $\epsilon_1(\delta)\leqq\epsilon$. Thus, if $0<\epsilon_2<\epsilon$, $q(\delta)\leqq\pi-\epsilon_2$ for sufficiently small δ. Now assume that, for a certain $i\geqq 1$ and real y, x, ξ,

$$|K^{(i)}(y,x;z)|\leqq 2^i\frac{\lambda_1+\delta}{(\lambda_1-\delta)^2}(\pi-\epsilon_2)^{i-1}. \tag{B12}$$

Then,

$$|K^{(i+1)}(y,x;z)|=\left|\int_{-1}^{1}K^{(i)}(y,\xi;z)K(\xi,x;z)d\xi\right|\leqq 2^i\frac{\lambda_1+\delta}{(\lambda_1-\delta)^2}(\pi-\epsilon_2)^{i-1}\int_{-1}^{1}\frac{2(\lambda_1+\delta)d\xi}{(\lambda_1-\delta)^2+(\xi-x)^2},$$

and

$$\int_{-1}^{1}\frac{2(\lambda_1+\delta)d\xi}{(\lambda_1-\delta)^2+(\xi-x)^2}=\frac{2(\lambda_1+\delta)}{(\lambda_1-\delta)}\int_{-1}^{1}\frac{(\lambda_1-\delta)d\xi}{(\lambda_1-\delta)^2+(\xi-x)^2}\leqq 2q(\delta)\leqq 2(\pi-\epsilon_2);$$

thus, (B12) holds for $i+1$. As shown above, (B12) does hold for $i=1$, and by induction it follows that (B12) holds for all $i\geqq 1$. As a consequence, the Neumann series (B11b) with $\lambda=z$ converges uniformly with respect to z in $\bar{D}$. The kernel K and its iterates are analytic functions of z in $\bar{D}$ because $\bar{D}$ does not intersect the imaginary axis, the only place where K and its iterates could have singularities. Thus, for $\sigma\geqq 1/2\pi$, (B11b) represents a uniformly converging series of analytic functions and, as a consequence,[13] $\kappa(y,x;z)$ is analytic in z in the neighborhood of any $\lambda_1>0$. In particular, κ is analytic in λ in the real sense. Finally, from (B11a) follows the analyticity of $g(y)$ as a function of λ. This completes the proof of statement (b) of Sec. III, that is $g(y)$ is analytic in λ for $\sigma=1/2\pi$.

[9] G. A. Campbell and R. M. Foster, *Fourier Integrals for Practical Applications* (American Telephone and Telegraph Company, New York, 1942), p. 45.
[10] Reference 7, p. 112.
[11] Reference 8, p. 270.
[12] Reference 7, p. 119.
[13] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, New York, 1952), p. 91.

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(iv) Using $1/(1+4a^2)\leqq|R(s,t)|\leqq 1$ and inequality (B7) one can prove by induction that

$$[1/(1+4a^2)](\pi/2)^{i-1}\leqq|R^{(i)}(s,t)|\leqq(\pi-\epsilon)^{i-1}.$$

Thus, there exist constants, b_1 and b_2, such that, for $\mu\leqq 1/\pi$,

$$0<b_1=[1/(1+4a^2)]\frac{1}{1-\mu(\pi/2)}\leqq|\rho(s,t)|$$

$$\leqq\frac{1}{1-\mu(\pi-\epsilon)}=b_2<\infty \quad \text{(B.13)}$$

If there exist constants b_3 and b_4 such that $b_3\leqq v(s)\leqq b_4$, then one obtains from (B10)

$$b_3(1+2ab_1)\leqq u(s)\leqq b_4(1+2a\mu b_2), \quad \text{(B14)}$$

which proves statement (d) of Sec. III, that is if $r(y)$ is bounded above or below, then so is the solution $g(y)$. The proof of statement (c) of Sec. III [that is, if $r(y)$ is positive definite, then so is the solution $g(y)$] follows immediately from (B14) as b_3 can be chosen positive in this case.

II. Numerical Solution

The basic integral equation (B2) has been solved numerically by applying Simpson's rule to the integral on a grid $\{s_i=-a+(i-1)h;\ h=a/n;\ i=1,\cdots,2n+1\}$. This yields a system of $(2n+1)$ linear algebraic equations for the $(2n+1)$ discrete approximate values $u_i\approx u(s_i)$ which can be solved by a standard method. The quadratures involved in calculating γ and e also have been carried out by Simpson's rule. The functions $K(\gamma)$ and $e(\gamma)$ are obtained in parametric form, that is $(K(\lambda),\gamma(\lambda))$ and $(e(\lambda),\gamma(\lambda))$. To obtain μ, the quantities e and γ are evaluated on a sufficiently fine grid of equidistant λ values. Then,

$$\mu=3e-\gamma\frac{de}{d\gamma}=3e-\gamma\frac{de}{d\lambda}\Big/\frac{d\gamma}{d\lambda}$$

can be calculated by numerical differentiation.

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Exact Analysis of an Interacting Bose Gas. II. The Excitation Spectrum

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We continue the analysis of the one-dimensional gas of Bose particles interacting via a repulsive delta function potential by considering the excitation spectrum. Among other things we show that: (i) the elementary excitations are most naturally thought of as a double spectrum, not a single one; (ii) the velocity of sound derived from the macroscopic compressibility is shown to agree with the velocity of sound derived from microscopic considerations, i.e., from the phonon spectrum. We also introduce a distinction between elementary excitations and quasiparticles, on the basis of which we give some heuristic reasons for expecting the double spectrum to be a general feature, even in three dimensions, and not an exception.

I. INTRODUCTION

IN the preceding paper[1] we introduced a soluble model of a Bose gas interacting via a repulsive δ-function potential. We discussed the nature of the eigenfunctions and explicitly calculated the ground-state energy and other properties of the ground state in the limit of a large system.

In this paper we discuss the nature of the excitation spectrum for a large system of N particles. The surprising result, as we stated but did not show in I, is that for all values of the potential strength, the most convenient and natural way to view the spectrum is to regard it as a *double* spectrum of elementary boson excitations. While Bogoliubov's perturbation theory[2,3] gives one of the spectra quite accurately for a weak potential, the second spectrum is entirely unaccounted for (see Figs. 3 and 4). The second spectrum exists only for values of the momentum satisfying $|p| \leq \pi\rho$.

We may summarize the results of this paper as follows: (i) In Sec. II we discuss the nature of the energy spectrum of the problem and show that there are two elementary spectra. These are always well defined and are explicitly calculated. We show that there is no energy gap and that the two spectra have a common slope at $p=0$ which means that they propagate sound at the same velocity. The velocity of sound at absolute zero derived in this way from an atomic picture[4–6] is shown to be identical with the velocity of sound defined by the usual macroscopic considerations [cf. Eqs. (1.1) and (1.4)].

[1] E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963) (referred to here as I).
[2] See I, Sec. IV.
[3] See, for example, *The Many Body Problem*, edited by C. DeWitt (John Wiley & Sons, Inc., New York, 1958), pp. 347–355.
[4] R. P. Feynman, Phys. Rev. **91**, 1291 (1953).
[5] R. P. Feynman, Phys. Rev. **91**, 1301 (1953).
[6] R. P. Feynman, Phys. Rev. **94**, 262 (1954).

The velocity of sound v_s, derived from the excitation spectrum is given by

$$v_s=\lim_{p\to 0}\partial\epsilon(p)/\partial p, \tag{1.1}$$

where $\epsilon(p)$ is the energy of an elementary excitation of momentum p. By a well-known macroscopic argument,[7] on the other hand,

$$v_s=[(-L/m\rho)\partial P/\partial L]^{1/2}, \tag{1.2}$$

where P is the pressure,

$$P=-\partial E_0/\partial L, \tag{1.3}$$

L is the length of the "box," $\rho=N/L$ is the density, m is the mass per particle ($=\frac{1}{2}$ in our units), and E_0 is the ground-state energy.

In I we defined the dimensionless parameter $\gamma=\rho^{-1}c$, where $2c$ is the strength of the δ function. In terms of γ, E_0 may be written $E_0=N\rho^2e(\gamma)$. In terms of these quantities, v_s may be written

$$\begin{aligned} v_s&=2\rho(3e-\gamma\dot{e}+\tfrac{1}{2}\gamma^2\ddot{e})^{1/2}\\ &=2(\mu-\tfrac{1}{2}\gamma\dot{\mu})^{1/2}, \end{aligned} \tag{1.4}$$

where "dot" denotes differentiation with respect to γ and μ is the chemical potential given by

$$\mu=\frac{\partial E_0}{\partial N}=\rho^2(3e-\gamma\dot{e}). \tag{1.5}$$

Bogoliubov's formula for $\epsilon(p)$ [I(4.1)] gives

$$v_s=2\rho\gamma^{1/2}, \tag{1.6}$$

while using Eq. (1.4) and Bogoliubov's expression for $e(\gamma)$[I(4.2)] we get

$$v_s=2\rho[\gamma-(1/2\pi)\gamma^{3/2}]^{1/2}. \tag{1.7}$$

Equations (1.6) and (1.7) are plotted as dashed curves in Fig. 5 along with the correct result for v_s obtained numerically. It will be noted that Eq. (1.7) is far more accurate than Eq. (1.6). In fact, the difference between Eq. (1.7) and the exact answer is so minute up to $\gamma=10$ that we are unable to distinguish the two graphically. This is indeed remarkable in view of the fact that Bogoliubov's expression for $e(\gamma)$ is quite bad beyond $\gamma=3$ and becomes negative for $\gamma>(3\pi/4)^2\simeq 5.5$.

(ii) Based on the results of this model, we are led to the introduction of two distinct quantities—called elementary excitations and quasiparticles—which are defined differently, and are, in fact, different, but which are apparently somehow related. This is discussed in Sec. III.

The quantities that we calculate are given by the solutions to certain integral equations. While these cannot be obtained in closed form we are able to prove directly the statements made above. The quantitative results have been obtained by Werner Liniger on an IBM 7090 computer at the IBM Research Center. The equations considered here are similar to those considered in I. The reader is referred to Appendix B of that paper for a discussion of the numerical methods employed.

[7] See, for example, F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II, p. 83.

II. EXCITED STATES AND ELEMENTARY EXCITATIONS

In paper I we discussed the Hamiltonian[8]

$$H=-\textstyle\sum_1^N\partial^2/\partial x_i^2+2c\sum_{(i,j)}\delta(x_i-x_j), \tag{2.1}$$

and showed that in the subdomain $0\leq x\leq\cdots\leq x_N\leq L$ all eigenfunctions are of the form

$$\psi(x_1,\cdots,x_N)=\textstyle\sum_P a(P)P\exp(i\sum_{j=1}^N k_jx_j), \tag{2.2}$$

where the summation is over permutations, P, of $\{k\}=k_1,<k_2,<\cdots,<k_N$, and $a(P)$ is a function of P. We found that for any set $\{k\}$ the $a(P)$'s could be uniquely determined. The condition determining the allowed k's is

$$\delta_j\equiv(k_{j+1}-k_j)L=\sum_{s=1}^{N}(\theta_{sj}-\theta_{sj+1})+2\pi n_j \qquad (j=1,2,\cdots,N-1) \tag{2.3}$$

$$\theta_{sj}=-2\tan^{-1}[(k_s-k_j)/c], \tag{2.4}$$

and n_j are any integers ≥ 1.

The ground state was obtained from Eq. (2.3) by putting all $n_j=1$. In this case $-k_1=k_N=K$ where K is a function of γ. The simplest excitation is obtained by putting some one $n_j=2$ while the rest remain unity. The effect of this is to increase δ_j by approximately 2π, but at the same time all the other δ's will be shifted slightly. Neglecting the change in spacing, the effect of making $n_j=2$ can be approximately thought of either as moving k_{j+1} to K (or $-K$) leaving a hole behind, or else as pushing apart the k's, leaving a double space at the jth position.

To orient ourselves, let us consider the $\gamma=\infty$ (hard core) case. As Girardeau[9] has pointed out, the energy spectrum of the Bose gas is then exactly the same as for a noninteracting one-component Fermi gas (the wave functions are quite different of course). The problem is this: How can we describe this Fermi spectrum in conventional boson terms? If we regard the energy levels simply as a collection of numbers, the problem is similar to that of classical spectroscopy. Can we find a small number of elementary energy levels from which all others may be deduced by addition?

The conventional description of the Fermi spectrum is to regard the elementary excitation process as taking a particle from the state q ($|q|<K$) to a state k ($|k|>K$). The energy and momentum of this state are

$$\begin{aligned} \epsilon(k,q)&=k^2-q^2,\\ p(k,q)&=k-q. \end{aligned} \tag{2.5}$$

[8] $\hbar=1$, $2m=1$.

[9] M. Girardeau, J. Math. Phys. 1, 516 (1960).

The difficulty with this classification scheme is twofold: (a) Every excitation must be described in terms of two parameters instead of merely one as one normally hopes to do for a Bose system. There is no unique $\epsilon(p)$ curve. (b) Too many provisos must be added to the original specification (e.g., there can be at most one excitation of any given type; $|q|$ can be greater than K for high-level compound excitations, etc.).

If we are interested only in low-lying excitations, however, difficulties (a) and (b) above can be remedied by the following scheme. Define two types of one parameter elementary excitations by these rules:

Type I. Take a particle from K to $q>K$ (or alternatively from $-K$ to $q<-K$). This excitation has an energy and momentum given by

$$\epsilon_1=q^2-K^2, \tag{2.6}$$

$$\begin{aligned} p&=q-K, \quad q>K \\ &=q+K, \quad q<-K \end{aligned} \tag{2.7}$$

$$\epsilon_1(p)=p^2+2\pi\rho|p|. \tag{2.8}$$

Type II. Take a particle from $0<q<K$ to $K+2\pi/L$ (or alternatively from $-K<q<0$ to $-K-2\pi/L$). The energy and momentum for this state are given to $O(N^{-1})$ by

$$\epsilon_2=K^2-q^2, \tag{2.9}$$

$$\begin{aligned} p&=K-q, \quad 0<q<K \\ &=-K-q, \quad 0>q>-K \end{aligned} \tag{2.10}$$

$$\epsilon_2(p)=2\pi\rho|p|-p^2. \tag{2.11}$$

For the first type of excitation $-\infty<p<\infty$ while for the second type $-\pi\rho\leq p\leq\pi\rho$ only. These two types of excitations must be supplemented by exactly two other excitations, which we shall call *umklapp* excitations, namely take a particle from $-K$ to $K+2\pi/L$ (or alternatively from K to $-K-2\pi/L$). The energies of the umklapp excitations are $2\pi^2\rho/L$ and, hence, are of order N^{-1}. Their momenta, however, are $2\pi\rho$ and $-2\pi\rho$, respectively.

Any of these excitations may be carried out any number of times and we may simultaneously have as many different types of as many different momenta as we please. For example, one type I excitation of momentum p means taking a particle from K to $K+p$. Two excitations of this same momentum means taking one more particle from $K-2\pi/L$ to $p-2\pi/L$. The momentum of the resulting state is exactly $2p$ while the energy is twice that of one excitation to order N^{-1}. Thus, each of these elementary excitations may be regarded as bosons.

By experimenting with a k-space diagram, the reader may easily convince himself that for any specified combination of multiple excitations of type I (or type II) there corresponds exactly one true state of the system, and conversely. The momentum of the true state is exactly the sum of the momenta of the elementary excitations, while the energy of the true state differs from the sum of the elementary energies only by $O(N^{-1})$ if the total number of excitations is finite (i.e., not of order N).

The difficulty with this classification scheme is that *either* type I *or* type II excitations form a "complete set" in the sense that they are in a one-one correspondence with the true excitation spectrum. Thus, any type II excitation may be thought of as a multiple type I excitation. The correspondence is this: m excitations of type I with momentum $p=2\pi n/L$ corresponds to exactly the same true state as n type II excitations with momentum $p=2\pi m/L$. In particular, one type II excitation of momentum p corresponds to $(1/2\pi)Lp$ type I excitations of momentum $p=2\pi/L$. If p is a fixed momentum independent of L, however, then the corresponding type II excitation may be thought of essentially as an infinite number of type I excitations of vanishing momentum. Since $\epsilon_1(p)$ and $\epsilon_2(p)$ are not proportional to p, the true energy of the type II excitation, $2\pi\rho p-p^2$, is very badly approximated by the $(1/2\pi)Lp$ type I excitations, viz.,

$$(1/2\pi)Lp[2\pi\rho(2\pi/L)-(2\pi/L)^2]\cong 2\pi\rho p.$$

The situation is, indeed, rather complicated and there does not seem to be any very simple way out of the dilemma. On the one hand, one can say that there is only one elementary excitation spectrum (one can choose either type I or type II) which is boson-like and which "generates" all the true states. On the other hand, physical considerations tell us that type I and type II excitations ought to stand on an equal footing, just as holes and particles play a similar role in the theory of the Fermi gas. It is patently absurd to think of a type II excitation as an infinite number of type I excitations of vanishing momentum.

We shall adopt here the "symmetric" point of view which seems to us the more natural way to view the problem. But we must then realize that if we calculate the partition function on this basis we will be double counting. The true free energy is that of the Fermi gas which one can calculate by standard methods. To leading order,

$$F=E_0-(kT)^2A, \tag{2.12}$$

where A is given by a well-known integral. If one calculates the free energy using the double boson spectrum [Eqs. (2.9) and (2.11)], one finds that

$$F'=E_0-2(kT)^2A. \tag{2.13}$$

The factor 2 is a precise reflection of the double counting. Either type I or type II alone would give Eq. (2.12). But if one does not double count, one gets a thoroughly distorted view of the nature of the excitation spectrum.

The situation for $\gamma\neq\infty$ is qualitatively the same as for the $\gamma=\infty$ case we have just discussed. Only the $\epsilon(p)$ functions differ; having discussed the over-all structure of the elementary excitations, we proceed now to calculate $\epsilon_1(P)$ and $\epsilon_2(P)$ for $\gamma\neq\infty$.

Type I Excitations ("Particle" States)

We put $n_j=1 (1\leq j\leq N-2)$ and $n_{N-1}\gg 1$. Let $k_N=q$, where $q>K$, and write

$$k_i'=k_i+(1/L)\omega_i, \quad i=1,\cdots,N-1 \qquad (2.14)$$

where k_i' are the new values of the remaining k's. At this point there are two ways to proceed—both leading of the same result. In Eq. (2.14) we could let $k_i=k$'s in the N-particle ground state, or we could let $k_i=k$'s in the $N-1$ particle ground state (ω_i will, of course, be different in the two cases). We shall adopt the latter definition because it leads to a simpler calculation.

Now,

$$\theta(k_j'-k_i')=\theta(k_j-k_i)+\frac{1}{L}(\omega_j-\omega_i)\frac{-2c}{c^2+(k_j-k_i)^2}. \qquad (2.15)$$

Inserting Eq. (2.15) in Eq. (2.3) or I(2.15) we obtain the integral equation

$$\omega(k)+\pi=2c\int_{-K}^{K}\frac{[\omega(r)-\omega(k)]f(r)}{c^2+(r-k)^2}dr-\theta(q-k), \qquad (2.16)$$

where $f(k)$ is the distribution function of the k's in the ground state, [cf. I(3.12)]. We have chosen the term π (instead of 3π, 5π, etc.) in Eq. (2.16) so that as $q\to 0$ the wave function approaches the ground-state wave function for N particles. If we define

$$\omega(k)f(k)\equiv J(k), \qquad (2.17)$$

Eq. (2.16) becomes

$$2\pi J(k)=2c\int_{-K}^{K}\frac{J(r)dr}{c^2+(k-r)^2}-\pi-\theta(q-k). \qquad (2.18)$$

Using Eq. (2.14) the momentum of the state is

$$P=\sum_{j=1}^{N-1}k_j'+q=\sum_{1}^{N-1}k_i+\frac{1}{L}\sum_{1}^{N-1}\omega_i+q$$
$$=q+\int_{-K}^{K}J(k)dk, \qquad (2.19)$$

while the excitation energy is

$$\epsilon_1=\textstyle\sum_{j=1}^{N-1}(k_i')^2-E_0(N)+q^2$$
$$=-\mu+q^2+2\int_{-K}^{K}kJ(k)dk, \qquad (2.20)$$

where $E_0(N)$ is the ground-state energy for N particles. To find $\epsilon_1(p)$ we have to eliminate the parameter q between Eqs. (2.19) and (2.20).

As we stated in I, Sec. III, Eq. (2.18) has a solution which is unique and negative definite (because $\pi+\theta(q-k)$ is positive definite). Since J (and, hence, ω) are negative we conclude, as was to be expected, that adding a particle with momentum $q>K$ to the $N-1$ particle system decreases all the other k's.

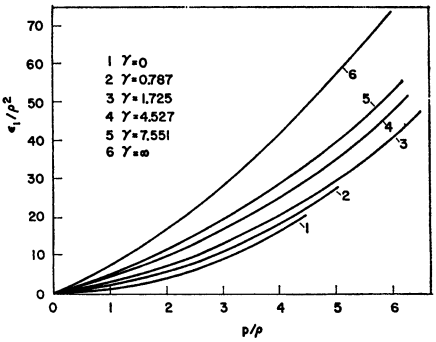

FIG. 1. The type I excitation spectrum, $\epsilon_1(p)$, plotted for small momenta and various values of $\gamma=c/\rho$. When $\gamma=0$, $\epsilon_1=p^2$; when $\gamma=\infty$, $\epsilon_1=p^2+2\pi\rho|p|$.

In Fig. 1 we display the $\epsilon_1(p)$ curve for several values of γ (in dimensionless units). The $\gamma=0$ curve is $\epsilon_1(p)=p^2$ (free particles), while the $\gamma=\infty$ is given by Eq. (2.8). All curves are linear for small p, the region of linearity increasing with γ.

The continuation of these curves for large p is given in the logarithmic plot of Fig. 2. To find an analytic expression for $\epsilon_1(p)$ for large p we expand $\theta(q-k)$ in a Laurent series for large q and retain the leading term. The obvious results are

$$J(k)\simeq-\frac{2\gamma\rho}{q}f(k), \qquad (2.21)$$

$$p\simeq q-2\gamma\rho^2/q, \qquad (2.22)$$

$$\epsilon_1(p)\simeq-\mu+p^2+4\gamma\rho^2. \qquad (2.23)$$

It should be noted that these last equations are true only if γ is finite and $p/\rho\gg\gamma$. If $\gamma=\infty$ on the other

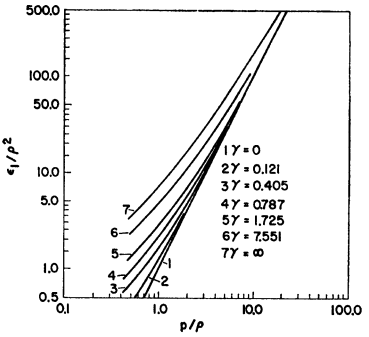

FIG. 2. The type I excitation spectrum for large momentum and various values of $\gamma=c/\rho$. When $\gamma=0$, $\epsilon_1=p^2$; when $\gamma=\infty$, $\epsilon_1=p^2+2\pi\rho|p|$.

hand, $\theta \equiv 0$ and Eqs. (2.6)–(2.8) must be used instead. In this case $J(k) = -\pi f(k) = -\frac{1}{2}$.

Equation (2.21) and (2.23) have a simple physical interpretation. The wave function can be well represented (in an average sense) by

$$\psi_p = \sum_P e^{ipx_N} \psi_0{}^{N-1}(x_1, \cdots, x_{N-1}), \qquad (2.24)$$

where the summation is on permutations and ψ_0 is the ground state for $N-1$ particles. In second-quantized notation this would be

$$\psi_p = a_p{}^\dagger |\psi_0{}^{N-1}\rangle. \qquad (2.25)$$

The energy of this state [Eq. (2.23)] can be interpreted as follows: First, remove a particle from the N-particle ground state. This contributes an energy—μ. Second, put it back in a plane wave state with momentum p—thereby adding p^2 to the energy. But the plane wave also interacts with the remaining $N-1$ particles—this energy is $\rho v(0)$ [$v(p)$ is the Fourier transform (F.T.) of the potential]. In our case this is $2\gamma\rho^2$. Finally, when the wave function is symmetrized, additional terms appear which ordinarily vanish as $p \to \infty$. But one of these terms—the F. T. of the potential times the two-particle correlation function—does not vanish for a δ-function and is in fact just $2\gamma\rho^2$. The total result is Eq. (2.23).

Before turning to excitations of type II ("hole" states) there are several questions to be answered about the behavior of Eqs. (2.18)–(2.20) as $q \to K$.

(a) Do both p and ϵ_1 vanish in this limit? If so, is $\epsilon_1(p)$ linear for small p?

(b) Is Bogoliubov's expression for the velocity of sound correct for small γ?

(c) Do the two expressions, Eqs. (1.1) and (1.4), for the velocity of sound agree for all γ?

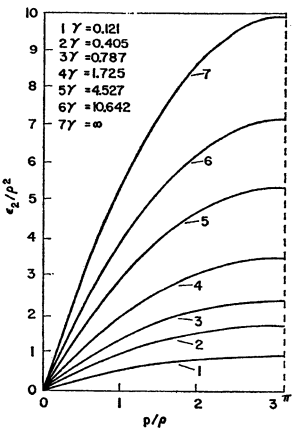

FIG. 3. The type II excitation, ϵ_2, as a function of momentum for various values of $\gamma = c/\rho$. This spectrum exists only up to $|p| = \pi\rho$. When $\gamma = 0$, $\epsilon_2 = 0$; when $\gamma = \infty$, $\epsilon_2 = -p^2 + 2\pi\rho|p|$.

All these questions can be answered in the affirmative, but the proof involves very tedious manipulation of the integral Eqs. I (3.18) and (2.18). These are summarized in the Appendix. Question (b) above is especially significant in view of the great debate as to whether or not there is an energy gap in the excitation spectrum. In our model there is none.

Type II Excitations ("Hole" States)

In this case we set all $n_i = 1$ except for $i = j$ when $n_j = 2$. Let $k_j = q$ (which we may assume to be a continuous parameter) with $0 < q < K$. In analogy with Eq. (2.14) we write

$$\begin{aligned} k_i' &= k_i + (1/L)\omega_i, \quad (i \leq j) \\ k_i' &= k_{i+1} + (1/L)\omega_i, \quad (i > j) \end{aligned} \qquad (2.26)$$

where now $k_i = k$'s in the $(N+1)$ particle ground state.

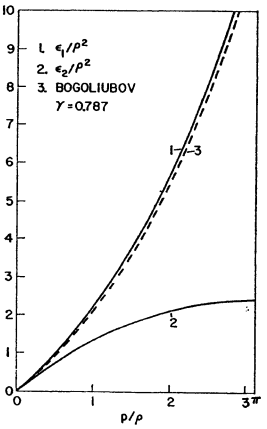

FIG. 4. A comparison plot of the two types of excitations, ϵ_1 and ϵ_2, for $\gamma = 0.787$. The dashed curve is Bogoliubov's spectrum which is quite close to the type I spectrum. The type II spectrum does not exist in Bogoliubov's theory.

As before we derive the equations

$$2\pi J(k) = 2c \int_{-K}^{K} \frac{J(r)dr}{c^2 + (k-r)^2} + \pi + \theta(q-k), \qquad (2.27)$$

$$p = -q + \int_{-K}^{K} J(k)dk, \qquad (2.28)$$

$$\epsilon_2 = \mu - q^2 + 2\int_{-K}^{K} kJ(k)dk. \qquad (2.29)$$

We observe that in this case $J(k)$ is negative definite (to see why this ought to be so, look at the $\gamma = \infty$ limit). When $q = K$, the solution to Eq. (2.27) is the negative of the solution to Eq. (2.18) so that in this limit both p and ϵ_2 vanish. As q decreases both p and ϵ_2 increase until, when $q = 0$, $p = \pi\rho$ [and not $K(\gamma)$ as might have been expected]. The case $q < 0$ need not be considered.

If we think of the Fermi case, what we have done is taken a particle from $q>0$ to K. Taking a particle from $q<0$ to K is, in our picture, to be regarded as the sum of two excitations; taking a particle from $q<0$ to $-K$ followed by an umklapp from $-K$ to K.

In Fig. 3 we show the $\epsilon_2(p)$ curves for various values of γ. The $\gamma=\infty$ case is given by Eq. (2.11). When $\gamma=0$, $\epsilon_2(p)\equiv 0$. Figure 4 compares $\epsilon_1(p)$, $\epsilon_2(p)$ and Bogoliubov's spectrum given in I Eq. (4.1) for $\gamma=0.787$. It will be seen that Bogoliubov's spectrum is a good approximation to $\epsilon_1(p)$ for this value of γ. It will also be noted that ϵ_1 and ϵ_2 have the same slope at $p=0$—a fact which may be easily proved from the integral equations. This common value of the velocity of sound is plotted in Fig. 5 together with Bogoliubov's results, Eqs. (1.6) and (1.7). With regard to the velocity of sound, we have seen that the macroscopic definition, Eq. (1.4), agrees for all γ with the microscopic definition based on the conjecture of Feynman[4–6] that the low-energy excitations are in general longitudinal phonons. But Feynman's additional conjecture that there is only one spectrum is apparently incorrect, at least in the present model. If one excites a sound wave in this system, most probably both types of excitations will be excited, just as in a Fermi gas both holes and particles are excited.

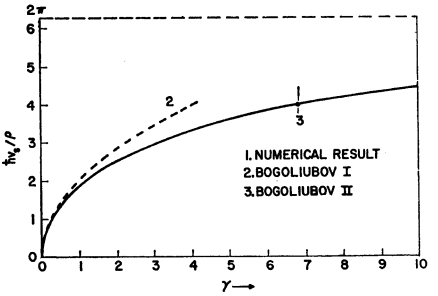

FIG. 5. The velocity of sound, v_s, as a function of $\gamma=c/\rho$. Curve 2 is the result obtained from Bogoliubov's excitation spectrum. Curve 3, which is graphically indistinguishable from the true result up to $\gamma=10$, is the velocity of sound derived from the macroscopic compressibility using Bogoliubov's expression for the ground-state energy.

III. A DISCUSSION OF ELEMENTARY EXCITATIONS AND QUASIPARTICLES

In the literature of the quantum-mechanical many-body problem two phrases are used interchangeably—elementary excitations and quasiparticles. We would like to propose here a distinction between the two.

A gas in a box has certain well-defined energies and wave functions which form a complete set. By definition these do not decay or interact with each other. The energies are real. Furthermore, as we have seen in our model and as is undoubtedly true, in general, the spectrum of low-lying states falls into a pattern. There exists one or more (in our case two) sets of energy vs momentum curves such that: (a) For each point on one of these curves there is an eigenstate; (b) if we add together the energy and momenta corresponding to several points on one or more of the curves, we obtain (to order N^{-1}) a resultant energy and momentum corresponding to an exact wave function of the system. The converse is also true: every state can be thought of as a sum of the elementary states.

These basic energy vs momentum curves we call *elementary excitations*. From this point of view, elementary excitations are a bookkeeping arrangement. There does not exist any simple operator which, acting on the ground state, gives these elementary states, nor can "compound" states be obtained from the elementary ones by simple operators. Nevertheless, when one attempts to diagonalize the many-body Hamiltonian by some method, it is the elementary excitations in the above sense that one is calculating.

Another quantity, called a *quasiparticle* may be defined as a pole in the Fourier transform of a propagator (or Green's function). The one-particle propagator is given in second quantized notation by[10] $G=G_+ + G_-$, where

$$G_+(p,t)=-i\langle\psi_0{}^N|\,a_p e^{-iHt}a_p{}^\dagger|\psi_0{}^N\rangle e^{iE_0t},\quad t>0,$$
$$G_-(p,t)=\pm i\langle\psi_0{}^N|\,a_p{}^\dagger e^{iHt}a_p|\psi_0{}^N\rangle e^{-iE_0t},\quad t<0, \qquad (3.1)$$

where the (+) sign is for fermions, the (−) sign for bosons. The time Fourier transform of both G_+ and G_- have a branch cut on the real axis and various singularities on the wrong Riemann sheet. The poles nearest the real axis are quasiparticle poles while the other singularities reflect more complex collective modes.

The energy of a quasiparticle (i.e., the position of the pole) is complex, which means that it decays in time. Nevertheless, there is a reputed connection, which has never been made very precise between quasiparticles and elementary excitations in the sense we have used them above. The difference between the two, and the reason one decays and the other does not, lies in the form of the wave functions. The elementary excitations refer to exact eigenfunctions which unfortunately, for an interacting system, do not have the plane wave character of the excitations of a noninteracting gas. The quasiparticle, on the other hand, may be thought of as an attempt to find (inexact) wave functions which do have a plane wave character. The function $a_p{}^\dagger|\psi_0{}^N\rangle$ in Eq. (3.1) is such a plane wave type function.

Elementary excitations are more useful for calculating the free energy or any other quantity where only the energy is involved. Quasiparticles are useful for calculating the response of the system to an external influence, for, by the nature of a physical excitation process, plane waves are generally excited at time $t=0$. The propagator G samples the exact states, so to speak, to find a linear combination which looks most like the plane wave state at $t=0$.

[10] V. M. Galitskii and A. B. Migdal, Soviet Phys.—JETP 7, 96 (1958).

For a noninteracting Bose gas, G_- is identically zero. The pole in G_+ lies on the real axis and gives the spectrum $\epsilon(p)=p^2$. When the interaction is turned on, the extent to which this pole moves off the real axis depends upon the extent to which $a_p^\dagger|\psi_0{}^N\rangle$ is no longer an exact eigenstate of the $N+1$ particle system. It is this pole to which perturbation based calculations direct their attention. In our case we have seen that for large p at least, $a_p^\dagger|\psi_0{}^N\rangle$ approaches an eigenstate [Eq. (2.25)]. Unfortunately, we are not in a position to calculate G, but if one believes that quasiparticle poles and elementary excitations are similar, than our $\epsilon_1(p)$ curve must be connected with this pole in G_+.

From whence arises our second spectrum, $\epsilon_2(p)$? We believe it is connected with G_-. The negative time part of the propagator must also have singularities, but since it vanishes for zero interaction it would be very difficult indeed for perturbation theory to find them. If $\phi_p=a_p|\psi_0{}^{N+1}\rangle$ were an exact eigenstate of the N-particle problem, G_- would have a pole on the real axis. For the noninteracting case $\phi_p\equiv 0$, but if we look at our type II wave functions it will be seen that to a rough approximation they are just ϕ_p. Thus, we are led to the view that our type II spectrum corresponds to a quasiparticle pole of the negative time part of the one body propagator.

We do not propose to elucidate here the connection between elementary excitations and quasiparticles—we merely point out that these two types of objects can be defined. Neither will we attempt to evaluate G. But the above discussion is pertinent to the outstanding question of whether our double excitation spectrum has any relevance in three dimensions.

It is to be noted, first of all, that all the quantities we have calculated are smoothly dependent on γ and behave just as one intuitively expects them to behave in any number of dimensions. Although we have frequently called attention to the analogy of this gas with a Fermi system, and although this Fermi gas analogy clearly breaks down in three dimensions, it should not be supposed that the double spectrum result is a consequence of one dimension forcing the Bose system to look like a Fermi system. While it may be argued that the salient difference between one and three dimensions is that in three dimensions particles can "get around each other," the true state of affairs is expressed by the functions $v(\gamma)$ and $t(\gamma)$ plotted in Fig. 1 of I. As we have already mentioned, the fact that the potential is effectively a kinetic energy barrier for large γ, a result that also holds in three dimensions, means that it is really immaterial to the particles whether they can "get around each other" or merely "through each other."

Thus, there appears to be no truly basic physical (as distinguished from mathematical) distinction between our gas and a similar gas in three dimensions. It is quite possible, therefore, that a double (or perhaps more fold) spectrum exists in three dimensions. Another possibility is that in three dimensions the double spectrum does not exist for small potentials, but makes its appearance when the potential becomes sufficiently strong. In the theory of a lattice of coupled harmonic oscillators,[11] for example, it is known that one imperfect light mass may cause an isolated energy level to appear above the perfect lattice band. In one dimension this always happens; in three dimensions it occurs only if the imperfect mass is sufficiently small. If this second possibility—the onset of a double spectrum for large potentials—were to occur, then clearly perturbation theory would be hard pressed to predict it.

We turn finally to an argument based on the previous considerations of this section. For the very same reasons that it is believed that the positive time part of the propagator has a pole near the real axis, the negative time part too may be presumed to have a similar pole. For what reason is this pole any less "elementary" than its counterpart in the positive time part of the propagator?

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APPENDIX: THE EXCITATION SPECTRUM AT LOW MOMENTUM AND THE VELOCITY OF SOUND

We justify here the claims made in Sec. II about the excitation spectrum of type I (a similar analysis applies to type II). We want to show the absence of a gap and the equivalence of the two definitions of v_s, Eqs. (1.1) and (1.4).

We first transform Eq. (2.18) to dimensionless form by defining

$$k=Kx;\quad J(Kx)=j(x);\quad q=Ks;\quad c=K\lambda;\quad \text{(A1)}$$

where $s\geq 1$. Expanding the inhomogeneous term in Eq. (2.18) for $s\sim 1$, we obtain

$$2\pi j(x)=2\lambda\int_{-1}^{1}\frac{j(y)dy}{\lambda^2+(x-y)^2}\pi+2\tan^{-1}\left(\frac{1-x}{\lambda}\right)+(s-1)\frac{2\lambda}{\lambda^2+(1-x)^2}. \quad \text{(A2)}$$

We write

$$j(x,s)=j_0(x)+(s-1)j_1(x), \quad \text{(A3)}$$

and define

$$2\phi_1(x)=j_0(x)+j_0(-x), \quad \text{(A4)}$$

$$2\phi_2(x)=j_0'(x)+j_0'(-x), \quad \text{(A5)}$$

$$2\phi_3(x)=j_1(x)+j_1(-x), \quad \text{(A6)}$$

$$2\phi_4(x)=j_1(x)-j_1(-x), \quad \text{(A7)}$$

[11] A. Maradudin, P. Mazur, E. Montroll, and G. Weiss, Rev. Mod. Phys. 30, 175 (1958).

where "prime" means differentiation with respect to x. We easily obtain the equations

$$2\pi\phi_1(x,\lambda)=\int \mathrm{Ker}\phi_1-\pi+\tan^{-1}\left(\frac{1-x}{\lambda}\right)+\tan^{-1}\left(\frac{1+x}{\lambda}\right), \quad \text{(A8)}$$

$$2\pi\phi_2(x,\lambda)=\int \mathrm{Ker}\phi_2-\lambda\left[\frac{1}{\lambda^2+(1-x)^2}+\frac{1}{\lambda^2+(1+x)^2}\right]\times[1+j_0(1)-j_0(-1)], \quad \text{(A9)}$$

$$2\pi\phi_3(x,\lambda)=\int \mathrm{Ker}\phi_3+\lambda\left[\frac{1}{\lambda^2+(1-x)^2}+\frac{1}{\lambda^2+(1+x)^2}\right], \quad \text{(A10)}$$

$$2\pi\phi_4(x,\lambda)=\int \mathrm{Ker}\phi_4+\lambda\left[\frac{1}{\lambda^2+(1-x)^2}-\frac{1}{\lambda^2+(1+x)^2}\right], \quad \text{(A11)}$$

where $\int$ Ker means the integral operator appearing in Eq. (A2).

The function $g(x,\lambda)$ introduced in I satisfies

$$2\pi g(x)=\int \mathrm{Ker}g+1, \quad \text{(A12)}$$

while the function

$$h(x,\lambda)=\left(\frac{\partial}{\partial\lambda}+\frac{x}{\lambda}\frac{\partial}{\partial x}\right)g \quad \text{(A13)}$$

satisfies

$$2\pi h(x)=\int \mathrm{Ker}h-2g(1,\lambda)\left[\frac{1}{\lambda^2+(1-x)^2}+\frac{1}{\lambda^2+(1+x)^2}\right]. \quad \text{(A14)}$$

A simple manipulation of Eq. (A12) shows that the function $g'=\partial g/\partial x$ satisfies

$$2\pi g'=\int \mathrm{Ker}g'-2\lambda g(1,\lambda)\left[\frac{1}{\lambda^2+(1-x)^2}-\frac{1}{\lambda^2+(1+x)^2}\right]. \quad \text{(A15)}$$

Comparing Eqs. (A10) and (A11) with Eqs. (A14) and (A15) we find that

$$\phi_3(x,\lambda)=-\frac{\lambda}{2g(1,\lambda)}h(x,\lambda), \quad \text{(A16)}$$

and

$$\phi_4(x,\lambda)=-\frac{1}{2g(1,\lambda)}g'(x,\lambda). \quad \text{(A17)}$$

Equation (A8) may be solved by inspection, i.e.,

$$\phi_1(x,\lambda)=-\tfrac{1}{2}. \quad \text{(A18)}$$

Comparison of Eqs. (A9) and (A10), together with the observation that

$$\int_{-1}^{1}dx\,\phi_2(x,\lambda)=j_0(1)-j_0(-1), \quad \text{(A19)}$$

yields the result

$$\phi_2(x,\lambda)=-\phi_3(x,\lambda)\left[1+\int_{-1}^{1}dx\,\phi_2(x,\lambda)dx\right]. \quad \text{(A20)}$$

Integrating Eq. (A14) with respect to x and using Eq. (A16) we find that

$$\int_{-1}^{1}dx\frac{\partial g}{\partial\lambda}=-\frac{2}{\lambda}g(1,\lambda)\left[1+\int_{-1}^{1}dx\,\phi_3(x,\lambda)\right]+\frac{1}{\gamma}, \quad \text{(A21a)}$$

$$\int_{-1}^{1}dx\,x^2\frac{\partial g}{\partial\lambda}=-\frac{2}{\lambda}g(1,\lambda)\left[1+\int_{-1}^{1}dx\,x^2\phi_3(x,\lambda)\right]+\frac{3}{\lambda}\int_{-1}^{1}dx\,x^2g(x,\lambda), \quad \text{(A21b)}$$

where we have used the definition of λ/γ given in I (3.20):

$$\frac{\lambda}{\gamma}=\int_{-1}^{1}dx\,g(x,\lambda)=\frac{\rho}{K}. \quad \text{(A22)}$$

Now, since

$$e(\gamma)=\frac{\gamma^3}{\lambda^3}\int_{-1}^{1}g(x,\lambda)x^2dx, \quad \text{(A23)}$$

[cf. I Eq. (3.19)], the definition of μ, Eq. (1.5) together with Eqs. (A21), is equivalent to

$$\mu=K^2\left[1+\int_{-1}^{1}dx\,\phi_3(x)x^2\right]\Big/\left[1+\int_{-1}^{1}dx\,\phi_3(x)\right]. \quad \text{(A24)}$$

In terms of the functions ϕ_1 to ϕ_4, Eq. (2.19) for the momentum takes the form (for $s\sim1$)

$$p=K\left[1+\int_{-1}^{1}dx\,\phi_1(x)\right]+K(s-1)\left[1+\int_{-1}^{1}dx\,\phi_3(x)\right]. \quad \text{(A25)}$$

The expression for ϵ_1, Eq. (2.20), takes the form (for $s\sim 1$)

$$\epsilon_1 = -\mu + K^2 + K^2\int_{-1}^{1} dx\,\phi_2(x)(1-x^2) + 2K^2(s-1)\left[1+\int_{-1}^{1} dx\,x\phi_4(x)\right] \quad \text{(A26)}$$

Inserting Eqs. (A18), (A20), and (A24) into Eqs. (A25) and (A26) we find that

$$\lim_{s\to 1} p = 0; \quad \lim_{s\to 1}\epsilon_1 = 0; \quad \text{(A27)}$$

thereby proving the assertion that there is no energy gap and that the lower end of the spectrum is in fact $p=0$.

Inserting Eqs. (A17) and (A22) into Eq. (A26), we find that for small s (i.e., small p)

$$\epsilon_1(p) = p\left\{g(1,\lambda)\left[1+\int_{-1}^{1} dx\,\phi_3(x)\right]\right\}^{-1}\rho. \quad \text{(A28)}$$

By Eq. (1.1), the velocity of sound, v_s, is, therefore, the factor $\{\ \}^{-1}\rho$ in Eq. (A28). It is always positive since ϕ_3 is positive. An alternative expression for v_s can be obtained from Eq. (A21a), viz.,

$$v_s = \frac{2}{\lambda}\left[\frac{1}{\gamma} - \int_{-1}^{1} dx\,\frac{\partial}{\partial\lambda}g(x,\lambda)\right]\rho. \quad \text{(A29)}$$

In I we showed that for λ small, $g(x,\lambda)\sim(1/2\pi\lambda)(1-x^2)^{1/2}$ and $4\lambda^2=\gamma$. Substituting this into Eq. (A29) we obtain

$$v_s \simeq 2\gamma^{1/2}\rho, \quad \text{(small } \gamma\text{)}, \quad \text{(A30)}$$

thereby confirming Bogoliubov's result, Eq. (1.6).

The last step is to confirm that Eqs. (1.4) and (A29) agree. We must calculate $d\mu/d\gamma = (d\lambda/d\gamma)(d\mu/d\lambda)$. The factor $d\lambda/d\gamma$ can be obtained from Eq. (A22) and (A21a), viz.,

$$\frac{d\lambda}{d\gamma} = \frac{1}{2}\frac{\lambda^2}{\gamma^2}\left\{g(1,\lambda)\left[1+\int_{-1}^{1} dx\,\phi_3(x)\right]\right\}^{-1}. \quad \text{(A31)}$$

To obtain $d\mu/d\lambda$ from Eq. (A24) the essential point is to evaluate $(\partial/\partial\lambda)\phi_3(x,\lambda)$. To this end we define the auxiliary function

$$m(x,\lambda) = \left(\frac{\partial}{\partial\lambda} + \frac{x}{\lambda}\frac{\partial}{\partial x}\right)\phi_3(x,\lambda). \quad \text{(A32)}$$

In analogy with Eqs. (A13) and (A14), this function satisfies

$$2\pi m(x,\lambda) = \int \mathrm{Ker} m - [1+2\phi_3(1,\lambda)]\left[\frac{1}{\lambda^2+(1-x)^2} + \frac{1}{\lambda^2+(1+x)^2}\right] + 2\left[\frac{1-x}{[\lambda^2+(1-x)^2]^2} + \frac{1+x}{[\lambda^2+(1+x)^2]^2}\right]. \quad \text{(A33)}$$

On the other hand, as we see from Eq. (A15), the function $g'' = \partial^2 g/\partial x^2$ satisfies

$$2\pi g'' = \int \mathrm{Ker} g - 2\lambda g'(1,\lambda)\left[\frac{1}{\lambda^2+(1-x)^2} + \frac{1}{\lambda^2+(1+x)^2}\right] - 4\lambda g(1,\lambda)\left[\frac{1-x}{[\lambda^2+(1-x)^2]^2} + \frac{1+x}{[\lambda^2+(1+x)^2]^2}\right]. \quad \text{(A34)}$$

Comparing Eqs. (A10), (A33), and (A34) we find that

$$m(x,\lambda) = -\frac{1}{2\lambda g(1,\lambda)}g''(x,\lambda) - \frac{1}{\lambda}\left[1+2\phi_3(1,\lambda)+\frac{g'(1,\lambda)}{g(1,\lambda)}\right]\phi_3(x,\lambda). \quad \text{(A35)}$$

In analogy with Eqs. (A21), $d\mu/d\lambda$ may be written in terms of $m(x,\lambda)$ which in turn may be written in terms of ϕ_3, g, g', and g'' by using Eq. (A35). We shall not carry out the tedious manipulation here, but one eventually finds that Eq. (1.4) reduces to Eq. (A29).

An alternative expression for v_s may be obtained by comparing Eqs. (A22), (A28), and (A31). One easily finds that

$$v_s = 2\rho\frac{\gamma^3}{\lambda^3}\frac{d\lambda}{d\gamma} = 2K - 2\gamma\frac{\partial K}{\partial\gamma}. \quad \text{(A36)}$$

Part XIII

One-Dimensional Hubbard Model

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Delta-Function Fermi Gas with Two-Spin Deviates*

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The problem of one-dimensional particles interacting via a delta-function potential has been a useful model for the many-body problem. While it can be solved for bosons, it has so far not been solved for fermions except for the special cases of either all spins parallel or all but one spin parallel. The full difficulty of the problem first manifests itself when two spins are down (i.e., $S=\frac{1}{2}N-2$), and this we solve here. We are confident that our method can be extended to the general problem.

INTRODUCTION

MANY authors have sought an exactly soluble model of interacting fermions (with ordinary pair potentials and in a "box" at a finite density) which would be an asset in the study of the many-body problem that pervades so much of physics.[1] Such a model—the delta-function model—exists for bosons,[2] but so far has defied solution for fermions. While there does exist one exactly soluble model of interacting fermions having physically reasonable properties,[3] the Hamiltonian of that model is sufficiently unphysical that it is difficult to have great confidence in its predictions.

In this paper we show how to solve the delta-function model for fermions with 2 spins down and $N-2$ spins up. We are fully confident that our method will solve the general problem, although its solution may be complicated. It must not be forgotten that one requires more of an exactly soluble model than a mere formal solution; one also needs an interpretation of the results. Since it is difficult to infer very much by comparison of the 2-spin deviate problem with the zero-spin deviate problem, we have put aside this important task until we are able to exhibit the full solution to the general problem.

The Hamiltonian[4] of the delta-function model for N particles is

$$H=-\sum_{1}^{N}\partial^2/\partial x_i^2+2c\sum_{1=i<j}^{N}\delta(x_i-x_j). \qquad (1.1)$$

Relative to bosons, fermions possess a simplifying as well as a complicating feature, the latter vastly outweighing the former. The simplification comes from the fact that an antisymmetric spatial wave function automatically vanishes when two particles "touch," so that the delta-function interaction plays no role. Thus, fermions with all spins parallel do not interact with each other. For other values of the total spin there will, indeed, be an interaction between the "spin-up" particles and the "spin-down" particles. In the latter case the problem is quite similar to the problem of a two-component Bose gas having the property that particles of each species interact only with particles of the other species. For particles of only one species (i.e., either a totally symmetric or a totally antisymmetric wave function), it is only necessary to consider the subregion of configuration space

$$R_1: \quad x_1\leq x_2\leq\cdots\leq x_N \qquad (1.2)$$

instead of the full configuration space because knowledge of the wave function in R_1 is, by symmetry, sufficient to define the wave function everywhere.

The complication mentioned above is that we are forced to consider a region much more complicated than R_1. To be explicit, suppose we wish to consider the eigenfunctions of H when j spins are down and $N-j$ spins are up [i.e., the value of S_z is $M_j=\frac{1}{2}(N-2j)$]. As was explained elsewhere,[5] it is necessary and sufficient to consider wave functions of the form $\Psi(x_1, x_2, \cdots, x_j \mid x_{j+1}, \cdots, x_N)$, where the "bar" means that Ψ is antisymmetric in the first j variables and in the last $N-j$ variables, but has no particular symmetry with respect to interchange of variables across the bar. Such a function could belong to a total $S\geq M_j$. Indeed,

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[1] For a review of exactly soluble many-body problems see E. Lieb and D. C. Mattis, *Mathematical Physics in One-Dimension* (Academic Press Inc., New York, 1966).

[2] E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963); E. Lieb, *ibid.* **130**, 1616 (1963).

[3] This model, based on the Thirring model of field theory was introduced by J. Luttinger, J. Math. Phys **4**, 1154 (1963), and was solved by D. C. Mattis and E. Lieb, *ibid.* **6**, 304 (1965).

[4] $\hbar=1$, $2m=1$.

[5] E. Lieb and D. C. Mattis, Phys. Rev. **125**, 164 (1962).

all functions belonging to $S \geq M_j$ have a representative in the M_j subspace by application of S_-, the spin-lowering operator. Thus, if we specify j (in this paper we shall consider $j=0$, 1, 2) there are two ways to determine the total S value of any particular wave function. The first, and complicated, way is to investigate the symmetry properties across the bar (i.e., to decide to which irreducible representation of the symmetric group the function belongs). The second, and simpler way, is to inquire whether the energy of Ψ is among the energies belonging to the $j-1$ subspace. If it does, then, barring accidental degeneracy, the S value of Ψ is greater than M_j.

To find eigenfunctions of the j type we must consider the configurational subspace

$$R^j: \quad x_1 \leq x_2 \leq \cdots \leq x_j, \qquad x_{j+1} \leq \cdots \leq x_N. \tag{1.3}$$

Equation (1.3) defines only a partial ordering. Plainly the region R^j contains $\binom{N}{j}$ physically distinguishable, completely ordered subregions of the type R_1. Herein lies the difficulty.

The imposition of periodic boundary conditions (PBC) does mitigate the difficulty somewhat, and we shall henceforth adopt these boundary conditions. Clearly, in this case, only the *relative* ordering of the "up" variables and the "down" variables is of any consequence. Thus, we need consider only $\binom{N-1}{j-1}$ essentially inequivalent subregions. For $j=1$, the case solved by McGuire,[6,7] it is only necessary to consider one instead of N regions. The full difficulty of the problem does not manifest itself until $j=2$. By solving this last case, we believe we shall be able to undertake the general problem of arbitrary j.

To solve the problem, we observe that the delta functions in (1.1) can be replaced by the $\binom{N}{2}$ boundary conditions:

$$\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)\Psi\,|_{x_i=x_i{}^+}-\left(\frac{\partial}{\partial x_i}-\frac{\partial}{\partial x_j}\right)\Psi\,|_{x_i=x_i{}^-}=2c\Psi\,|_{x_i=x_j}, \tag{1.4a}$$

together with the continuity conditions

$$\Psi\,|_{x_i=x_i{}^+}=\Psi\,|_{x_i=x_i{}^-}. \tag{1.4b}$$

These are in addition to the periodic boundary conditions (PBC):

$$\Psi(x_1, \cdots, x_j, \cdots, x_N)=\Psi(x_1, \cdots, x_j+L, \cdots, x_N) \tag{1.5}$$

for $j=1, 2, \cdots, N$. Here, L is the length of the "box." It is obviously sufficient to restrict our attention, whatever the order of the x's, to

$$x_{\max}-x_{\min} \leq L, \tag{1.6}$$

and we shall do so henceforth. We then make the following *Ansatz* for Ψ: For a suitable choice of N *distinct* numbers $\{k\}=k_1, k_2, \cdots, k_N$, we note that Ψ can be written in every subregion R_α of the type R_1 as

$$\psi_\alpha(x_1, \cdots, x_N)=\sum_P A_\alpha(P)\,\exp(i\sum_1^N k_{j(P)}x_j), \tag{1.7}$$

where $\sum_P$ stands for a sum on $N!$ permutations. The important point to note is that $A_\alpha(P)$ is a set of coefficients which depend upon the particular region R_α, but that the set $\{k\}$ is fixed and does not depend upon R_α. The problem is to find the allowed sets $\{k\}$, together with their accompanying coefficients $\{A_\alpha(P)\}$ such that the boundary conditions (1.4) and (1.5) are satisfied.

Clearly, the Schrödinger differential equation is satisfied with an energy

$$E=\sum_1^N k_i{}^2. \tag{1.8}$$

Moreover, the total momentum of the state will be

$$P=\sum_1^N k_i, \tag{1.9}$$

and we know that any allowed set $\{k\}$ will automatically satisfy

$$P=(2\pi/L)\times\text{integer}. \tag{1.10}$$

Before investigating the $j=2$ case, let us see how the program works for $j=0$ and $j=1$. For $j=0$, we need consider only R_1 (1.2) and impose the boundary condition that $\psi=0$ on the boundary of R_1. In an arbitrary subregion, R_α, $\psi_\alpha=\pm\psi_1$ and it is seen that the continuity conditions and delta-function conditions (1.4) will be automatically satisfied. The PBC, (1.5), reads

$$\begin{aligned}\Psi(x_1, \cdots, x_j, \cdots, x_N) &=\Psi(x_1, \cdots, x_j+L, \cdots, x_N)\\ &=(-1)^{N-j}\Psi(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_N, x_j+L)\end{aligned} \tag{1.11}$$

for all $j=1, \cdots, N$. The point of Eq. (1.11) is that the PBC has been reduced to a statement about Ψ in R_1 alone, i.e., about ψ_1. Now, the fact that ψ_1 vanishes on the boundary of R_1 implies that $A_1(P)=\epsilon_P$, whence

$$\psi_1(x_1, \cdots, x_N)=\text{Det}\,|\,\exp ik_i x_j\,|. \tag{1.12}$$

Equation (1.11) then fixes the k_i as

$$k_i=(2\pi/L)n_i, \tag{1.13}$$

where $n_1, \cdots, n_N$ is any set of distinct integers. The

[6] J. B. McGuire, J. Math. Phys. 6, 432 (1965).
[7] J. B. McGuire, J. Math. Phys. 7, 123 (1966).

result then, for the $j=0$ case, is that the eigenfunctions and eigenvalues are the same as for the noninteracting case. In fact, as we could have seen in advance, (1.12) represents Ψ everywhere, not only in R_1, but this is fortuitous; it will not be true for $j>0$.

For $j=1$, the region R^1, Eq. (1.3) consists of N regions $R_1, R_2, \cdots, R_N$ where R_k is defined by the fact that $x_k \leqq x_1 \leq x_{k+1}$. As we remarked above, the PBC imply that these N regions are effectively equivalent. Using PBC we can find enough conditions in R_1 alone to determine $\{k\}$. Denoting the value of Ψ in R_i by ψ_i, and using PBC on the "up" particles, we have

$$\begin{aligned}\psi_2(x_1 \mid x_2, x_3, \cdots, x_N) &= \psi(x_1 \mid x_2+L, x_3, \cdots, x_N) \\ &= (-1)^{N-2}\psi_1(x_1 \mid x_3, x_4, \cdots, x_N, x_2+L).\end{aligned} \tag{1.14}$$

It is here that the value of PBC manifests itself, for we now have two conditions connecting R_1 and R_2; (1.4) and (1.14). These, together with (1.10), are sufficient to determine $\{k\}$.

Since ψ_1 vanishes whenever $x_{j+1}=x_j$ ($j=2, \cdots, N-1$), we obviously infer

$$\psi_1 = \begin{vmatrix} f_1\chi_{11} & f_2\chi_{12} & \cdots & f_N\chi_{1N} \\ \chi_{21} & \chi_{22} & \cdots & \chi_{2N} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ \chi_{N1} & \chi_{N2} & \cdots & \chi_{NN} \end{vmatrix}, \tag{1.15}$$

where $f_1, \cdots, f_N$ are some coefficients and

$$\chi_{ij} \equiv \exp(ix_ik_j).$$

If we denote by $D_{mn}(x_3, \cdots, x_N)$ the cofactor of $f_m\chi_{1m}\chi_{2n}$ in the determinant of Eq. (1.15), and use the fact that ψ_2 vanishes whenever $x_{j+1}=x_j$ ($j=3, \cdots, N-1$), then

$$\psi_2 = \sum_{m,n=1} A_{mn}\chi_{1m}\chi_{2n}D_{mn}(x_3, \cdots, x_N). \tag{1.16}$$

In this language, the $j=0$ case is retrieved by the choice $f_j=1$ and $A_{mn}=1$ (all j, m, n).

The delta-function condition, (1.4a), reads

$$i(k_n-k_m)(f_m+f_n-A_{mn}-A_{nm}) = 2c(f_m-f_n), \tag{1.17a}$$

while the continuity condition, (1.4b), reads

$$f_m-f_n = A_{mn}-A_{nm} \tag{1.17b}$$

for all $m \neq n$. Finally, the PBC reads

$$A_{mn} = f_m \exp(ik_nL). \tag{1.18}$$

Inserting Eq. (1.18) into Eq. (1.17), we find

$$f_m(1-\chi_n) = ic(f_n-f_m)/(k_n-k_m), \tag{1.19}$$

where $\chi_n = \exp(ik_nL)$. One solution is to have $\chi_n=1$ and $f_n=1$ (all n), thereby recovering the $j=0$ solution. Otherwise, by comparing Eq. (1.19) to the same equation with n and m interchanged, we find

$$f_n = (1-\chi_n). \tag{1.20}$$

Upon insertion of Eq. (1.20) into Eq. (1.19) and a small amount of algebraic manipulation, we have

$$\tfrac{1}{2}c \cot\tfrac{1}{2}(k_jL) - k_j = \lambda \tag{1.21}$$

(λ a constant), with the constraint that $k_n \neq k_m$. This is the famous equation first derived by McGuire[6] and discussed extensively by him.[6,7] It is useful to rewrite Eq. (1.21) as

$$\chi_j = \frac{k_j+\lambda+\frac{1}{2}(ic)}{k_j+\lambda-\frac{1}{2}(ic)}. \tag{1.22}$$

The reader will note that for every pair of neighboring regions, R_j and R_{j+1}, there is a similar pair of boundary conditions [i.e., Eq. (1.4) and the analog of Eq. (1.14)], and he can easily verify that these will be satisfied by the same choice of $\{k\}$ as in (1.21). Where the final condition, Eq. (1.10), enters is in the PBC on the "down" particle, x_1:

$$\begin{aligned}\psi_1(x_1 \mid x_2, \cdots, x_N) &= \psi(x_1+L \mid x_2, \cdots, x_N) \\ &= \psi_N(x_1+L \mid x_2, \cdots, x_N),\end{aligned} \tag{1.23}$$

an equation connecting R_1 to R_N. This will be satisfied for the choice (1.21) if and only if (1.10) is obeyed. It is clear from Eq. (1.22) that Eq. (1.10) may be rewritten as

$$\prod_{j=1}^{N} \left(\frac{k_j+\lambda+\frac{1}{2}(ic)}{k_j+\lambda-\frac{1}{2}(ic)}\right) = 1 \tag{1.24}$$

Finally, it must be remembered that the solutions to Eq. (1.22) and Eq. (1.24) give only the $S_{\text{total}} \geq \frac{1}{2}N-1$ states for the Hamiltonian (1.1). The $S_{\text{total}}=\frac{1}{2}N$ states correspond to $\lambda=\infty$.

The final result is startling. It is that each k_j satisfies an "independent particle" equation, (1.21), which is only slightly more complicated than that for the noninteracting gas, (1.13). True, these equations are not really independent because the separation constant λ in Eq. (1.21) must be chosen to satisfy the momentum condition (1.10). Nevertheless, the situation is much simpler than for the Bose gas[2] where each k is a function of all the other k's.

When $j=2$, the algebraic problem will be vastly more complicated than the foregoing because we must consider $(N-1)$ inequivalent subregions rather than one subregion. Nevertheless, the final equations for $\{k\}$ bear a striking similarity to Eqs. (1.22) and (1.24).

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It is the main purpose of this paper to prove that

$$\chi_j \equiv \exp(ik_jL) = \left(\frac{k_j+\delta+\frac{1}{2}(ic)}{k_j+\delta-\frac{1}{2}(ic)}\right)\left(\frac{k_j+\epsilon+\frac{1}{2}(ic)}{k_j+\epsilon-\frac{1}{2}(ic)}\right), \tag{1.25}$$

where

$$\prod_{j=1}^{N}\left(\frac{k_j+\delta+\frac{1}{2}(ic)}{k_j+\delta-\frac{1}{2}(ic)}\right)=\frac{\epsilon-\delta-ic}{\epsilon-\delta+ic}, \tag{1.26a}$$

$$\prod_{j=1}^{N}\left(\frac{k_j+\epsilon+\frac{1}{2}(ic)}{k_j+\epsilon-\frac{1}{2}(ic)}\right)=\frac{\delta-\epsilon-ic}{\delta-\epsilon+ic}. \tag{1.26b}$$

Here, δ and ϵ are two constants. Once again, solutions to (1.25) and (1.26) give us only the $S_{\text{total}} \geq \frac{1}{2}N-2$ states.

II. THE TWO-SPIN DEVIATE PROBLEM—DETERMINATION OF $\{k\}$

The region R^2, Eq. (1.3), contains $\binom{N}{2}$ primitive subregions which we shall denote by R_{jk}, the index j signifying the position of x_1 among the N variables and the index k signifying the position of x_2 measured from x_1. Thus

$$\begin{aligned} R_{11}&: \ x_1<x_2<x_3<x_4<\cdots<x_N, \\ R_{12}&: \ x_1<x_3<x_2<x_4<\cdots<x_N, \\ R_{21}&: \ x_3<x_1<x_2<x_4<\cdots<x_N, \ \text{etc.} \end{aligned} \tag{2.1}$$

The regions R_{1k} $(k=1, \cdots, N-1)$ are the fundamental inequivalent regions, for our intuition tells us, although we must carefully verify it explicitly, that all regions with a common value of the second index are equivalent to each other. Each region R_{jk} is connected to neighboring regions through Eq. (1.4). For $k>1$ and $j>1$ there are four: $R_{j-1,k+1}$, $R_{j+1,k-1}$, $R_{j,k+1}$, and $R_{j,k-1}$. For $k=1$ and $j>1$ there are two: $R_{j-1,k+1}$ and $R_{j,k+1}$.

Our first step will be to take a "down" particle through the "up" particles. That is, if we assume we know $\psi_{1,1}$ then Eq. (1.4) will determine $\psi_{1,2}$ and then $\psi_{1,3}$, etc. Finally, $\psi_{1,1}$ is related to $\psi_{1,N-1}$ by PBC:

$$\begin{aligned} \psi_{1,1}(x_1x_2 \mid x_3, \cdots, x_N) &= \psi(x_1+L, x_2 \mid x_3, \cdots, x_N) \\ &= -\psi(x_2, x_1+L \mid x_2, \cdots, x_N) \\ &= -\psi_{1,N-1}(x_2, x_1+L \mid x_3, \cdots, x_N). \end{aligned} \tag{2.2}$$

We shall then be able to determine a great deal, but not everything, about $\{k\}$. The remaining conditions will come later from the second step—taking an "up" particle through the "down" particles.

Since $\psi_{1,1}$ vanishes when $x_1=x_2$ or when $x_{j-1}=x_j$ $(j=4, \cdots, N)$, we have

$$\psi_{1,1}=\tfrac{1}{2}\sum_{s,t=1,s\neq t}^{N} A(st) f_{st}(x_1, x_2) D_{st}(x_3, \cdots, x_N), \tag{2.3}$$

where

$$f_{st}(x_1x_2)=\chi_{1s}\chi_{2t}-\chi_{1t}\chi_{2s} \tag{2.4}$$

and D_{st} is as previously defined [Eq. (1.15) *et seq.*]. Obviously, $A(st)=A(ts)$. Likewise, define

$$D_{stu\cdots}=\text{cofactor of } \chi_{1s}\chi_{2t}\chi_{3u}\cdots \tag{2.5}$$

in the determinant of Eq. (1.12). The wave function in $R_{1,j-1}$ can be written (for $j=3, \cdots, N$) as

$$\psi_{1,j-1}=\sum_{\substack{\alpha_1\cdots\alpha_j=1 \\ \text{(all distinct)}}}^{N} A^{j-1}(\alpha_1, \cdots, \alpha_j) \times \prod_{m=1}^{j}\chi_{m,\alpha_m} D_{\alpha_1,\cdots,\alpha_j}(x_{j+1}, \cdots, x_N). \tag{2.6}$$

The fact that $\psi_{1,j-1}$ vanishes when $x_{m-1}=x_m$ (for $m=4, 5, \cdots, j-2$) requires that $A^{j-1}(\alpha_1, \cdots, \alpha_j)$ be *symmetric* in the last $j-2$ variables. Beyond that there is no other symmetry requirement on A^j.

Just as we derived Eq. (1.17),[8] we can use (1.4) to express A^{j-1} in terms of A^{j-2}, viz.,

$$\begin{aligned} A^{j-1}(\alpha_1, \cdots, \alpha_j) &= A^{j-2}(\alpha_1, \cdots, \alpha_{j-1})[1-ic(k_{\alpha_2}-k_{\alpha_j})^{-1}] \\ &+A^{j-2}(\alpha_1, \alpha_j, \alpha_3, \cdots, \alpha_{j-1})\,(ic)\,(k_{\alpha_2}-k_{\alpha_j})^{-1}, \end{aligned} \tag{2.7}$$

where $A^1(\alpha_1, \alpha_2) \equiv A(\alpha_1, \alpha_2)$. Defining

$$t(r, s)=-ic(k_r-k_s)^{-1} \quad \text{and} \quad m(r, s)=1+t(r, s), \tag{2.8}$$

we deduce that

$$A^{j-1}(\alpha_1, \cdots, \alpha_j)=A(\alpha_1, \alpha_2)\prod_{k=3}^{j} m(\alpha_2, \alpha_k) + \sum_{k=3}^{j} A(\alpha_1, \alpha_k) t(\alpha_k, \alpha_2) \prod_{l=3, l\neq k}^{j} m(\alpha_k, \alpha_l). \tag{2.9}$$

The last product in Eq. (2.9) is to be omitted for $j=3$. The derivation of Eq. (2.9) from Eq. (2.7) is a simple exercise in induction if one observes that

$$t(k, l)\,t(m, k)+t(l, k)\,t(m, l)+t(m, k)\,t(l, m)=0. \tag{2.10}$$

Note that A^{j-1} satisfies the symmetry requirements mentioned above.

To determine $A(s, t)$ we turn to the PBC relation, (2.2), which states that

$$A(s, t)=\chi_s A^{N-1}(t, s, \alpha_3, \cdots, \alpha_N) \tag{2.11}$$

[8] For details such as this, see Michael Flicker, Ph.D. thesis, Yeshiva University, 1966 (unpublished).

for t, s not in the set $\alpha_3, \cdots, \alpha_N$, and with $\chi_s = \exp(ik_sL)$ as before. We insert (2.9) into (2.11) and using (2.8) and a bit of algebraic manipulation we obtain the key equation

$$\sum_{j=1}^{N} (K_{sj} - K_{rj}) B_{jr} = 0 \tag{2.12}$$

for all $s, r = 1, \cdots, N$. Here,

$$K_{sj} = \delta_{sj}\chi_s^{-1} - ic\eta_j(k_s - k_j + ic)^{-1}, \tag{2.13a}$$

$$\eta_j = \prod_{k=1, k\neq j}^{N} m_{jk}, \tag{2.13b}$$

$$B_{sj} = A(s,j)(k_s - k_j). \tag{2.13c}$$

A necessary and sufficient condition for $A(s,j)$ to be symmetric is that B_{sj} be antisymmetric. Even though $A(s,s)$ is not defined, we have defined $B_{ss} = 0$ in obtaining (2.12). Furthermore, if $k_j = k_s + ic$ for some pair s and j, then K_{sj} is not well defined by (2.13a). In such a case, however, $\eta_j = 0$ and it is correct to use L'Hospital's rule whence

$$-ic\eta_j(k_s - k_j + ic)^{-1} \text{ is replaced by } \prod_{k=1, k\neq j, k\neq s}^{N} m_{jk}.$$

Equation (2.12) can be regarded as an eigenvalue equation for the antisymmetric matrix B. Only for special choices of K, and hence of $\{k\}$, will there be a solution. To solve (2.12) for B we first regard the N-dimensional vector $\mathbf{P}$, defined by

$$P_r = \sum_j K_{rj} B_{jr}, \tag{2.14}$$

as a known vector, and then determine B from the matrix equation

$$\sum_j K_{sj} B_{jr} = P_r. \tag{2.15}$$

If $\mathbf{P} = 0$, then (2.15) is homogeneous. Let $\mathbf{V}^1, \mathbf{V}^2, \cdots, \mathbf{V}^\mu$ be an orthonormal basis for the null space, V, of K, which is defined as the set of vectors satisfying

$$K\mathbf{V} = 0. \tag{2.16}$$

Then, for a fixed r, we can write

$$B_{jr} = \sum_{\alpha=1}^{\mu} V_j^\alpha S_r^\alpha, \tag{2.17}$$

where the S_r^α are a set of μ coefficients which depend upon r. But, since B is antisymmetric, it is easy to prove that (for $\mathbf{P} = 0$)

$$B_{jr} = \sum_{\alpha=1}^{\mu} \sum_{\beta=1}^{\mu} V_j^\alpha V_r^\beta C_{\alpha\beta}, \tag{2.18}$$

where C is *any* antisymmetric μ-square matrix. Of course, $\mu = d(V) =$ dimension of V is unknown. Unless $\mu \geq 2$, there is no solution to (2.15) for $\mathbf{P} = 0$.

If $\mathbf{P} \neq 0$, then multiply (2.15) by P_r^* and sum on r. Defining the vector $\mathbf{G} = B\mathbf{P}^*$, we have

$$K\mathbf{G} = \rho^2\mathbf{I}, \tag{2.19}$$

where $\mathbf{I}$ is the vector $I_j = 1$ and $\rho^2 = \sum_r |P_r|^2 \neq 0$. This means that the matrix K must have a "unit vector" $\mathbf{g}$:

$$K\mathbf{g} = \mathbf{I}. \tag{2.20}$$

This unit vector can be defined to be orthogonal to the space V and hence is unique. By the same argument as that leading to (2.18), it is easy to show that

$$B_{jr} = \sum_\alpha \sum_\beta V_j^\alpha V_r^\beta C_{\alpha\beta} + g_j P_r - P_j g_r. \tag{2.21}$$

If this form is inserted into (2.15), it follows at once that $\mathbf{P}$ must itself be a null vector which may be taken to be $\rho\mathbf{V}^1$. Hence, the general solution to (2.15) is

$$B_{jr} = \sum_{\alpha=1}^{\mu} \sum_{\beta=1}^{\mu} V_j^\alpha V_r^\beta C_{\alpha\beta} + \rho(g_j V_r^1 - V_j^1 g_r). \tag{2.22}$$

If now we recall the definition of $\mathbf{P}$ [Eq. (2.14)], we see that for arbitrary ρ and arbitrary antisymmetric C (2.22) is indeed a solution to (2.12).

In conclusion, we may state that the necessary and sufficient conditions for a nonzero antisymmetric solution, B, to (2.12) to exist is that the matrix K have either (a) a "unit vector" and one or more null vectors or (b) no unit vector but two or more null vectors. In both cases, the general solution is (2.22).

At this point we could inquire into the properties of $\{k\}$ necessary to insure that the above requirement on K is fulfilled. Since it turns out that the set $\{k\}$ is *not* thereby completely determined, we shall instead turn to additional properties of B which will completely determine $\{k\}$. These are provided by the PBC on the "up" particles.

Consider first the *full* statement of PBC for the "down" particles which is that

$$\begin{aligned}\psi_{1j}(x_1, x_2 \mid x_3, \cdots, x_N) &= \psi(x_1 + L, x_2 \mid x_3, \cdots, x_N) \\ &= -\psi(x_2, x_1 + L \mid x_3, \cdots, x_N) \\ &= -\psi_{j,N-j}(x_2, x_1 + L \mid x_3, \cdots, x_N)\end{aligned} \tag{2.23}$$

for $j = 1, \cdots, N-1$. Equation (2.23) leads to Eq. (2.12) for $j = 1$, as we have already discussed, but for $j > 1$ it is first necessary to define $\psi_{j,N-j}$. This can be done from the statement of PBC on the "up" particles which reads

$$\begin{aligned}\psi_{ij}(x_1, x_2 \mid x_3, \cdots, x_N) &= \psi(x_1, x_2 \mid x_3 + L, x_4, \cdots x_N) \\ &= (-1)^{N-1}\psi_{i-1,j}(x_1, x_2 \mid x_4, \cdots, x_N, x_3 + L)\end{aligned} \tag{2.24}$$

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for $i=2, \cdots, N-1$. If we iterate (2.24) $i-1$ times, we obtain

$$\psi_{ij}(x_1, x_2 \mid x_3, \cdots, x_N) = (-1)^{(N-1)(i-1)}\psi_{1j}(x_1, x_2 \mid x_{i+2}, \cdots, x_N, x_3 + L, \cdots, x_{i+1}+L). \quad (2.25)$$

Equation (2.25) gives ψ_{ij} in terms of ψ_{1j} (for $i>1$) and, in fact, may be taken as the definition of ψ_{ij}. With this definition of ψ_{ij} it is trivial to verify that (a) PBC for the "up" particles, (2.24), is automatically satisfied and (b) the delta-function and continuity conditions, (1.4), relating the ψ_{ij} to each other are automatically fulfilled if the sequence ψ_{1j} satisfies these conditions. This latter requirement has already been met through (2.12).

Thus, the only outstanding condition to be satisfied is (2.23) which, using (2.25), reads

$$\psi_{1j}(x_1, x_2 \mid x_3, \cdots, x_N) = -(-1)^{(N-1)(j-1)}\psi_{1,N-j}(x_2, x_1+L \mid x_{j+2}, \cdots, x_N, x_3 + L, \cdots, x_{j+1}+L). \quad (2.26)$$

In terms of the functions A^j defined in (2.6), Eq. (2.26) becomes

$$A^j(\alpha_1, \cdots, \alpha_{j+1}) = A^{N-j}(\alpha_2, \alpha_1, \alpha_{j+2}, \cdots, \alpha_N)\chi_{\alpha_1}\prod_{i=3}^{j+1}\chi_{\alpha_i}. \quad (2.27)$$

Equation (2.27) must be satisfied for $j=1, \cdots, N-1$. It seems intuitively reasonable, however, that satisfying it for $j=1$ (as we have done) and for $j=2$ should be sufficient, because in some sense we will have thereby satisfied PBC for an "up" and a "down" particle. Unfortunately, we have not found a general proof with which to make our intuition rigorous. Instead, we give a tedious, but rigorous, inductive proof in Appendix A, using the defining Eq. (2.9), that (2.27) is automatically satisfied for all j if it is satisfied for $j=1$ and $j=2$.

To evaluate (2.27) for $j=2$, we insert the definitions (2.8), (2.9), and (2.13) and obtain

$$\frac{1}{\chi_r\chi_j}\left[\frac{B_{rs}m_{sj}}{k_r-k_s}+\frac{B_{rj}t_{js}}{k_r-k_j}\right] = ic\sum_{e=1}^{N}\frac{B_{se}(k_j-k_e)\eta_e}{(k_r-k_e+ic)(k_s-k_e+ic)(k_j-k_e+ic)} \quad (2.28)$$

for every triplet of distinct integers r, s, j. If we now make a partial fraction expansion of the triple product in the denominator of (2.28) and make use of the condition (2.12), we obtain the alternative condition

$$B_{sr}\{k_sk_r\alpha_j+k_s\beta_j+k_r\gamma_j+\delta_j\} = ic(k_r-k_s)\{B_{rj}+\chi_rB_{sj}\}, \quad (2.29)$$

where

$$\alpha_j = 1-\chi_j,$$
$$\beta_j = \chi_j(k_j-ic)-k_j,$$
$$\gamma_j = k_j\chi_j-(k_j+ic),$$
$$\delta_j = k_j^2(1-\chi_j)+ick_j(1+\chi_j). \quad (2.30)$$

It is a simple matter to show that (2.29) is true for *all* values of r, s, and j not only distinct values. Our problem is then completely solved if we can choose $\{k\}$ so that (2.22) and (2.29) are both satisfied.

Consider the four vectors, $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\delta}$ which are defined in (2.30). Note that $\boldsymbol{\gamma}=\boldsymbol{\beta}-ic\boldsymbol{\alpha}$. We wish to show that these vectors are in the space $U=V\oplus\mathbf{g}$ which is the set of all vectors $\mathbf{u}$ such that $K\mathbf{u}=$constant. To do this we consider the space Q orthogonal to U and show that $\boldsymbol{\alpha}\cdot\mathbf{q}=\boldsymbol{\beta}\cdot\mathbf{q}=\boldsymbol{\gamma}\cdot\mathbf{q}=\boldsymbol{\delta}\cdot\mathbf{q}=0$ for all $\mathbf{q}$ in Q. It is easy to show that Q is nonempty but it is not necessary to do so. If $\mathbf{q}$ is in Q, multiply (2.29) by q_j^* and sum on j. From (2.22) $B\mathbf{q}=0$, whence

$$B_{sr}\xi_{sr}=0 \qquad (\text{all } s, r), \quad (2.31)$$

where

$$\xi_{sr} = k_sk_r(\boldsymbol{\alpha}\cdot\mathbf{q})+k_s(\boldsymbol{\beta}\cdot\mathbf{q})+k_r(\boldsymbol{\gamma}\cdot\mathbf{q})+\boldsymbol{\delta}\cdot\mathbf{q}=0. \quad (2.32)$$

Now, B_{sr} can not be zero for all s and r (otherwise the wave function vanishes), and we can therefore state that $B_{\sigma\rho}\neq0$ for some σ and ρ. Since B is antisymmetric it follows that $B_{\rho\sigma}\neq0$ as well. We can also state that $B_{\tau\rho}\neq0$ for some $\tau\neq\sigma$ otherwise, from (2.15) $K_{s\sigma}B_{\sigma\rho}=P_\rho$ so that $K_{s\sigma}$ is independent of s—an impossible conclusion by inspection of (2.13a) and use of the fact that the k's are distinct. Hence, (2.31) says that $0=\xi_{\sigma\rho}=\xi_{\rho\sigma}=\xi_{\tau\rho}=\xi_{\rho\tau}$ for σ, ρ, and τ distinct. Again, using the fact that the k's are distinct, we conclude that the factors in parentheses in (2.32) are zero and we establish that $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\delta}$ are in U. Note that if $\mathbf{P}=0$, then $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\delta}$ are in V.

The above exploited only the properties of (2.29) and did not take into account the fact that the matrix K contains χ and is therefore not totally unrelated to the vectors $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\delta}$. We now make use of this latter fact and find the stronger result that $\boldsymbol{\alpha}$ and $\boldsymbol{\gamma}$ (and hence $\boldsymbol{\beta}$ also) must be contained in the null space V whether or not $\mathbf{P}=0$. To prove this we rewrite (2.13a) as $K_{sj}=\delta_{sj}\chi_s^{-1}+D_{sj}$ with

$$D_{sj} = -ic\eta_j(k_s-k_j+ic)^{-1}. \quad (2.33)$$

The matrix D has two interesting properties:

(a) $$\sum_j D_{sj} = -1; \tag{2.34}$$

(b) if $$\sum_j D_{sj} u_j = w_s, \tag{2.35a}$$

then

$$\sum_j D_{sj} u_j k_j = ic\left(\sum_j \eta_j u_j\right) + (k_s + ic) w_s. \tag{2.35b}$$

To prove (a) consider

$$F(x) \equiv \prod_{j=1}^{N} [1 - ic(x - k_j)^{-1}]$$

$$= 1 - ic \sum_{j=1}^{N} \eta_j (x - k_j)^{-1}, \tag{2.36}$$

the latter form having been obtained by partial fraction expansion. The first expression yields $F(k_s + ic) = 0$, while the second yields $F(k_s + ic) = 1 + \sum_j D_{sj}$, Q.E.D. The proof of (b) follows immediately from (2.33) and the observation that

$$u_j k_j = -u_j(k_s - k_j + ic) + u_j(k_s + ic).$$

Note that the first term on the right side of (2.35b) is a constant, independent of s, and is therefore proportional to the vector $\mathbf{I}$ introduced in (2.19).

To proceed, we introduce an abbreviated, self-explanatory, notation whereby a quantity such as $\mathbf{k}\alpha$ stands for the vector with components $k_j \alpha_j$, while χ^{-1} stands for the vector with components $(\chi_j)^{-1}$. Now, since α, γ, and δ are in $V \oplus \mathbf{g}$ we have

$$K\alpha = b^1 \mathbf{I},$$

$$K\gamma = b^2 \mathbf{I},$$

$$K\delta = b^3 \mathbf{I}, \tag{2.37}$$

where b^1, b^2, and b^3 are certain constants. To prove that α and γ are in V we must show that $0 = b^1 = b^2$. Using the explicit forms (2.30) we have

$$D\alpha = (b^1 + 1)\mathbf{I} - \chi^{-1}, \tag{2.38a}$$

$$D\gamma = b^2 \mathbf{I} - \mathbf{k} + (\mathbf{k} + ic)\chi^{-1}, \tag{2.38b}$$

$$D\delta = b^3 \mathbf{I} + \mathbf{k}(\mathbf{k} - ic) - \mathbf{k}(\mathbf{k} + ic)\chi^{-1}. \tag{2.38c}$$

But note that $\gamma = -\mathbf{k}\alpha - ic\mathbf{I}$ and, inserting this expression into (2.38b) and using lemmata (a) and (b) above, we have

$$D\gamma = -ic(b^1 + \sum_{j=1}^{N} \eta_j \alpha_j)\mathbf{I} - \mathbf{k} + (\mathbf{k} + ic)\chi^{-1} - b^1 \mathbf{k}. \tag{2.39}$$

Since the right sides of (2.38b) and (2.39) must be equal for all the N different values of k, we must conclude that $b^1 = 0$. Likewise, $\delta = -\mathbf{k}\gamma + ic\mathbf{k} - ic\mathbf{k}\alpha$. Inserting this into (2.38c) and again using the two lemmata, we have

$$D\delta = -\mathbf{k}(\mathbf{k} + ic)\chi^{-1} + \mathbf{k}(\mathbf{k} - ic) - b^3 \mathbf{k}$$

$$+ ic[ic \textstyle\sum \eta_j \chi_j - \sum \eta_j \gamma_j - 2ic - b^2]\mathbf{I}. \tag{2.40}$$

Upon comparison with the right side of (2.38c), we see that b^3 must also vanish, Q.E.D.

We note also that $b_1 = b_2 = 0$ implies, from (2.38b) and (2.39), that

$$\sum_{j=1}^{N} \eta_j \alpha_j = 0. \tag{2.41}$$

The condition that $K\alpha = K\beta = 0$ is thus equivalent to

$$K\alpha = 0 \text{ and } (2.41).$$

The next fact to be proved is that, for $S_T = \frac{1}{2}N - 2$, $B_{sr} = E_1(\alpha_s \beta_r - \alpha_r \beta_s)$ where E_1 depends on the normalization of the wave function. At the very end of the proof we make the important observation that δ is a linear combination of α and β and also that $\mathbf{P} = 0$. It will become clear during the course of the proof exactly how the possibilities $S_T = \frac{1}{2}N$, $S_T = \frac{1}{2}N - 1$, and $S_T = \frac{1}{2}N - 2$ come out of the formalism.

When we combine (2.29) and the equation obtained from it by interchange of r and s we obtain

$$B_{sr}\alpha_j = [B_{sj}\alpha_r - B_{rj}\alpha_s]. \tag{2.42}$$

If we now substitute the explicit form of B (2.22) into the right-hand side and also observe that when (2.42) is multiplied by K_{ls} and summed on s one obtains

$$\rho V_r{}^l \alpha_j = \rho V_j{}^l \alpha_r, \tag{2.43}$$

it then follows that

$$B_{sr}\alpha_j = \sum_i C_{ij}'(V_s{}^i \alpha_r - V_r{}^i \alpha_s) + \rho V_j{}^l(\alpha_r g_s - \alpha_s g_r), \tag{2.44}$$

where $C_{ij}' = \sum_k C_{ik} V_j{}^k$. Clearly there are now two possibilities for the α_j; either $\alpha_j = 0$ for all j or $\alpha_j \neq 0$ for some j. If $\alpha_j = 0$ for all j, then $S_T = \frac{1}{2}N$; we will not say any more about this possibility. If $\alpha_j \neq 0$ for some j, then from (2.44) we have

$$B_{sr} = E_1(\alpha_r \beta_s - \alpha_s \beta_r) + E_2(\alpha_r v_s - \alpha_s v_r) + E_3(\alpha_r g_s - \alpha_s g_r), \tag{2.45}$$

where $\mathbf{v}$ is a null vector orthogonal to α and β, and E_1, E_2, and E_3 are constants. Upon substitution of (2.45) into (2.29) it follows, after some algebra, that

$$B_{sr}(\mathbf{v} \cdot \delta) = icE_2 \mid v \mid^2 \{\alpha_r k_s + \beta_r + \chi_r(ic\alpha_s - \beta_s) - k_r \chi_r \alpha_s\}. \tag{2.46}$$

Recalling that $KB = \mathbf{P}$, $K\alpha = 0$, and $K\beta = 0$, we obtain from (2.46)

$$P_r(\mathbf{v} \cdot \delta) = icE_2 \mid v \mid^2 \{\alpha_r \sum_s K_{ls} k_s + \beta_r \sum_s K_{ls}\}. \tag{2.47}$$

Since a consequence of (2.43) is that $\mathbf{P}=\rho\sigma\alpha(\sigma\neq 0)$, either α and β are linearly dependent or

$$ic E_2 \mid v \mid^2 \beta_r \sum_s K_{ls}=0 \quad \text{for all} \quad r, l.$$

If the former is the case, then $S_T=\frac{1}{2}N-1$ (this is the solution of McGuire[6]). The remaining possibility corresponds to $S_T=\frac{1}{2}N-2$. It is a simple exercise to show that, for some l, $\sum_s K_{ls}\neq 0$. Also $\beta_r\neq 0$ for some r; if $\beta_r=0$ for all r, then α and β are linearly dependent and we have the McGuire problem. Hence $E_2 \mid v \mid^2=0$. In a similar way we conclude that $E_3=0$. Consequently $B_{sr}=E_1(\alpha_r\beta_s-\alpha_s\beta_r)$. Direct substitution of this relation into (2.29) verifies that δ is a linear combination of α and β; from (2.22) it is obvious that $\mathbf{P}=0$.

To summarize the results for $S_T=\frac{1}{2}N-2$:

(i) α and β are null vectors;

(ii) δ is a linear combination of α and β;

(iii) $B_{sr}=E_1(\alpha_r\beta_s-\alpha_s\beta_r)$.

What remains to be done is to put (i) and (ii) into a form more amenable to the calculation of the set $\{k\}$. From (ii) and (2.30) we obtain an equation that when solved for χ yields (1.25), i.e.,

$$\chi_j\equiv\exp(ik_jL)=\frac{[k_j+\delta+\frac{1}{2}(ic)]\,[k_j+\epsilon+\frac{1}{2}(ic)]}{[k_j+\delta-\frac{1}{2}(ic)]\,[k+\epsilon-\frac{1}{2}(ic)]}, \quad (2.48)$$

where δ and ϵ are constants to be determined. The assumption $\delta<\epsilon$ can be partially justified[8] by observing that the set $\{k_j(c)\}$ is one to one with the known set $\{k_j(0)\}$.

Having obtained the expression (2.48) for χ_j (and thus α and β) in terms of k_j, our problem will be completely solved if we can satisfy condition (i), namely that α and β be null vectors. This requirement leads to the conditions (1.26) on the constants δ and ϵ. The details are given in Appendix B.

III. THE ENERGY LEVELS

In this section we will derive the explicit form, in the thermodynamic limit, of the sets $\{k_j\}$. Once the $\{k_j\}$ are known, the determination of the energy levels is straightforward. As an illustration of this we will calculate the ground-state energy.

In order to calculate the sets $\{k_j\}$ it is helpful to write Eqs. (1.25) and (1.26) in a slightly different form. With the observation that

$$\frac{[k_j+\delta+\frac{1}{2}(ic)]}{[k_j+\delta-\frac{1}{2}(ic)]}=-\exp\{-2i\tan^{-1}(2/c)(k_j+\delta)\}, \quad (3.1)$$

we see that (1.25) is equivalent to

$$k_j+\frac{2}{L}\tan^{-1}\frac{2}{c}(k_j+\delta)+\frac{2}{L}\tan^{-1}\frac{2}{c}(k_j+\epsilon)=\frac{2\pi n_j}{L} \quad (3.2)$$

and (1.26) to

$$2\tan^{-1}\left(\frac{\epsilon-\delta}{c}\right)+2\sum\tan^{-1}\frac{2}{c}(k_j+\delta)=2\pi\nu+\pi[(N-1)\bmod 2], \quad (3.3a)$$

$$2\tan^{-1}\left(\frac{\delta-\epsilon}{c}\right)+2\sum\tan^{-1}\frac{2}{c}(k_j+\epsilon)=2\pi\mu+\pi[(N-1)\bmod 2]. \quad (3.3b)$$

In particular, we are interested in determining the energy levels in the limit of a large system. This means N, $L\to\infty$ such that $\rho=N/L=$fixed constant. Under these conditions the set $\{k_j\}$ can be determined by iteration. To determine the energy and momentum of a state correct to $O(1)$ it is sufficient that k be known to $O(1/L)$. It is clear from (3.2) that it is only necessary to know ϵ and δ to $O(1)$ to get the desired accuracy for k. However, from (3.3) it follows that it is only necessary to know the k's to $O(1)$ in order to get ϵ and δ to $O(1)$. This is because μ, ν will be $O(N)$ and the summation on the left hand side of (3.3) will be $O(N)$. But to $O(1)$, $k_j=2\pi n_j/L$, therefore ϵ and δ are the solutions to

$$\sum\tan^{-1}\frac{2}{c}\left(\frac{2\pi n_j}{L}+\delta\right)=\pi\nu, \quad (3.4a)$$

$$\sum\tan^{-1}\frac{2}{c}\left(\frac{2\pi n_j}{L}+\epsilon\right)=\pi\mu; \quad (3.4b)$$

and, to the desired accuracy,

$$k_j=\frac{2\pi n_j}{L}-\frac{2}{L}\tan^{-1}\frac{2}{c}\left(\frac{2\pi n_j}{L}+\delta\right)-\frac{2}{L}\tan^{-1}\frac{2}{c}\left(\frac{2\pi n_j}{L}+\epsilon\right). \quad (3.5)$$

Note: Since, for $c\neq 0$, the k's are distinct, the n's are also distinct.

The numbers $\{n_j\}$, μ, and ν, which clearly are the quantum numbers of the system and specify all the states, must be known in order to calculate the energy of any state. Therefore, the first step in calculating the ground-state energy must be to determine its quantum numbers. Since the k_j's are given essentially by $2\pi n_j/L$, the problem is similar to that of the one-dimensional noninteracting, spinless Fermi gas. Thus, we would expect $n_{j+1}-n_j=1$, $n_1\sim-[\frac{1}{2}N]$ and $n_N\sim[\frac{1}{2}N]$. The proof that this is actually the case is quite simple. Consider two states, a and b, such that

$$\begin{aligned} n_i^a&=n_i^b \qquad i=1,\cdots,j;\\ n_{i+1}^a&=n_i^b \qquad i=j+1,\cdots,N-1;\\ \nu_a&=\nu_b;\qquad \mu_a=\mu_b;\qquad \mid n_j^a\mid<\mid n_N^b\mid. \end{aligned} \quad (3.6)$$

From (3.4) it is clear that, to the order of interest, $\delta^a=\delta^b$ and $\epsilon^a=\epsilon^b$. Hence, from (3.5) it is obvious that

$|k_j^a|<|k_N^b|$. Since $E^b-E^a=(k_N^b)^2-(k_j^a)^2$ we conclude $E^a<E^b$. By induction it follows that in the ground state $n_{j+1}-n_j=1$. Thus,

$$n_j=-\tfrac{1}{2}(N-2j+1)+\lambda, \tag{3.7}$$

where $\lambda=0$ for N odd and $\lambda=\pm\frac{1}{2}$ for N even.

Define

$$q_j\equiv 2\pi n_j/L \tag{3.8}$$

then from (3.5)

$$k_j=q_j-(2/L)[\tan^{-1}(2/c)\,(q_j+\delta)+\tan^{-1}(2/c)\,(q_j+\epsilon)]. \tag{3.9}$$

Therefore, the energy, (1.8), of the state is given to $O(1)$ by

$$E=\sum_{j=1}^{N}\left\{q_j^2-\frac{4}{L}q_j\left[\tan^{-1}\frac{2}{c}\,(q_j+\delta)+\tan^{-1}\frac{2}{c}\,(q_j+\epsilon)\right]\right\}. \tag{3.10}$$

The term $\sum q_j^2$ is just the ground state for $S=N/2$. Thus, changing the remaining sum to an integral, (3.10) can be written as

$$E=E_g(S=\tfrac{1}{2}N)-\frac{2}{\pi}\int_{-K}^{K}q[\tan^{-1}(2/c)\,(q+\delta)+\tan^{-1}(2/c)\,(q+\epsilon)]dq, \tag{3.11}$$

where $K=\pi\rho$. When E is minimized with respect to ϵ and δ, we obtain the ground state energy for $S=\frac{1}{2}N-2$.

$$E_g(S=\tfrac{1}{2}N-2)=E_g(S=\tfrac{1}{2}N)+2c\rho-4\pi\rho^2\tan^{-1}\frac{2\pi\rho}{c}-\frac{c^2}{\pi}\tan^{-1}\frac{2\pi\rho}{c}. \tag{3.12}$$

The result is just what one would expect. The deviation from $E_g(S=N/2)$ is just twice the deviation of the $S=\frac{1}{2}N-1$ problem.[6]

APPENDIX A

Theorem: If

$$A^m(\alpha_1,\cdots,\alpha_{m+1})=A^{N-m}(\alpha_2,\alpha_1,\alpha_{m+2},\cdots,\alpha_N)\chi_{\alpha_1}\prod_{i=3}^{m+1}\chi_{\alpha_i} \tag{A1}$$

for $m=1$, 2 then it is true for $m>2$.

Proof: The proof is by induction. We will assume (A1) is true for $m=j-2$, $j-1$ and prove it is true for $m=j$.

The natural starting place is Eqs. (2.7) that relate various A^j's. To proceed: From (2.7) we obtain two equations, one that "steps down" the A^j's and another that "steps up" the A^j's, that is,

$$A^{j-1}(\alpha_1,\cdots,\alpha_{j+1})=A^{j-2}(\alpha_1,\cdots,\alpha_{j-1})m(\alpha_2,\alpha_j)-A^{j-2}(\alpha_1,\alpha_j,\alpha_3,\cdots,\alpha_{j-1})t(\alpha_2,\alpha_j), \tag{A2a}$$

$$A^{j-2}(\alpha_1,\cdots,\alpha_{j-1})=A^{j-1}(\alpha_1,\cdots,\alpha_j)m(\alpha_j,\alpha_2)-A^{j-1}(\alpha_1,\alpha_j,\alpha_3,\cdots,\alpha_{j-1},\alpha_2)t(\alpha_j,\alpha_2). \tag{A2b}$$

If we "step up" $A^{N-j}(\alpha_1,\cdots,\alpha_{N-j+1})$ and change the indices as follows

$$\begin{aligned}&\alpha_1\to\alpha_2\\ &\alpha_2\to\alpha_1\\ &\alpha_3\to\alpha_{j+2}\\ &\quad\cdots\\ &\alpha_{N-j+1}\to\alpha_N\\ &\alpha_{N-j+2}\to\alpha_{j+1},\end{aligned}$$

we obtain

$$A^{N-j}(\alpha_2,\alpha_1,\alpha_{j+2},\cdots,\alpha_N)=A^{N-j+1}(\alpha_2,\alpha_1,\alpha_{j+1},\cdots,\alpha_N)m(\alpha_{j+1},\alpha_1)-A^{N-j+1}(\alpha_2,\alpha_{j+1},\alpha_{j+2},\cdots,\alpha_N,\alpha_1)t(\alpha_{j+1},\alpha_1). \tag{A3}$$

Since (A1) is true for $m=j-1$, (A3) yields

$$\chi_{\alpha_1}\prod_{i=3}^{j+1}\chi_{\alpha_i}A^{N-j}(\alpha_2,\alpha_1,\alpha_{j+2},\cdots,\alpha_N)=\chi_{\alpha_{j+1}}m(\alpha_{j+1},\alpha_1)A^{j-1}(\alpha_1,\cdots,\alpha_j)-\chi_{\alpha_1}t(\alpha_{j+1},\alpha_1)A^{j-1}(\alpha_{j+1},\alpha_2,\cdots,\alpha_j). \tag{A4}$$

But, when we step down $A^j(\alpha_1,\cdots,\alpha_{j+1})$ we find

$$A^j(\alpha_1,\cdots,\alpha_{j+1})=A^{j-1}(\alpha_1,\cdots,\alpha_j)m(\alpha_2,\alpha_{j+1})-A^{j-1}(\alpha_1,\alpha_{j+1},\alpha_3,\cdots,\alpha_j)t(\alpha_2,\alpha_{j+1}). \tag{A5}$$

Thus, if (A1) is to be true for $m=j$ we must prove that

$$\text{r.h.s. (A4)}-\text{r.h.s. (A5)}\equiv\Lambda_{j-1}=0. \tag{A6}$$

If in (A6) we change variables to

$$\begin{aligned}\alpha_1&=r,\\ \alpha_2&=s,\\ \alpha_j&=u,\\ \alpha_{j+1}&=v,\\ \{(\alpha_3,\cdots,\alpha_{j+1})\}&=\alpha,\end{aligned}$$

With M. Flicker in Phys. Rev. *161*, 179–188 (1967)

and "step down" all A^{j-1}'s to A^{j-2}'s we obtain

$$\chi_v m(v,r)\{A^{j-2}(rs\alpha)m(s,u)-A^{j-2}(ru\alpha)t(s,u)\}$$
$$-\chi_v t(v,r)\{A^{j-2}(vs\alpha)m(s,u)-A^{j-2}(vu\alpha)t(s,u)\}$$
$$-m(s,v)\{A^{j-2}(rs\alpha)m(s,u)-A^{j-2}(ru\alpha)t(s,u)\}$$
$$+t(s,v)\{A^{j-2}(rv\alpha)m(v,u)-A^{j-2}(ru\alpha)t(v,u)\}$$
$$=\Lambda_{j-1}. \quad \text{(A7)}$$

Since (A1) is assumed true for $m=j-2, j-1$, it is obvious that $\Lambda_{j-2}=0$. As a consequence we have

$$\chi_v m(v,r)A^{j-2}(rs\alpha)-\chi_v t(v,r)A^{j-2}(vs\alpha)$$
$$-m(s,v)A^{j-2}(rs\alpha)=-A^{j-2}(rv\alpha)t(s,v) \quad \text{(A8a)}$$

and

$$\chi_v m(v,r)A^{j-2}(ru\alpha)-\chi_v t(v,r)A^{j-2}(vu\alpha)$$
$$=m(u,v)A^{j-2}(ru\alpha)-t(u,v)A^{j-2}(rv\alpha). \quad \text{(A8b)}$$

Direct substitution of (A8) into (A7) coupled with (2.10) require $\Lambda_{j-1}=0$ Q.E.D.

APPENDIX B

The condition that α is a null vector is

$$\sum_{j=1}^{N} K_{ij}(1-\chi_j)=0. \quad \text{(B1)}$$

In terms of the matrix D_{ij} defined in (2.33) plus the property (2.34) (B1) can be written as

$$\sum_{j=1}^{N} D_{ij}\chi_j=\chi_i^{-1}-2. \quad \text{(B2)}$$

But from (2.48)

$$\sum_{j=1}^{N} D_{ij}\chi_j=-ic\sum_{j=1}^{N}\frac{\eta_j}{(k_i-k_j+ic)}$$
$$\times\frac{[k_j+\delta+(\frac{1}{2}ic)][k_j+\epsilon+(\frac{1}{2}ic)]}{[k_j+\delta-(\frac{1}{2}ic)][k_j+\epsilon-(\frac{1}{2}ic)]}. \quad \text{(B3)}$$

Assuming $\epsilon\neq\delta$, we can make a partial fraction expansion of the triple product in (B3):

$$\frac{1}{(k_i-k_j+ic)}\frac{[k_j+\delta+(\frac{1}{2}ic)][k_j+\epsilon+(\frac{1}{2}ic)]}{[k_j+\delta-(\frac{1}{2}ic)][k_j+\epsilon-(\frac{1}{2}ic)]}$$
$$=\frac{[k_i+\delta+\frac{3}{2}(ic)][k_i+\epsilon+\frac{3}{2}(ic)]}{[k_i+\delta+(\frac{1}{2}ic)][k_i+\epsilon+(\frac{1}{2}ic)]}\frac{1}{(k_i-k_j+ic)}$$
$$+\frac{ic(ic+\epsilon-\delta)}{(\epsilon-\delta)[k_i+\delta+(\frac{1}{2}ic)]}\frac{1}{[k_j+\delta-(\frac{1}{2}ic)]}$$
$$+\frac{ic(ic+\delta-\epsilon)}{(\delta-\epsilon)[k_i+\epsilon+(\frac{1}{2}ic)]}\frac{1}{[k_j+\epsilon-(\frac{1}{2}ic)]}. \quad \text{(B4)}$$

If we define

$$a\equiv -ic\sum\eta_j[k_j+\delta-(\tfrac{1}{2}ic)]^{-1}$$

and

$$b\equiv -ic\sum\eta_j[k_j+\epsilon-(\tfrac{1}{2}ic)]^{-1}, \quad \text{(B5)}$$

and again use (2.34), then from (B3)

$$\sum_{j=1}^{N} D_{ij}\chi_j=-\frac{[k_i+\delta+(\frac{3}{2}ic)][k_i+\epsilon+(\frac{3}{2}ic)]}{[k_i+\delta+(\frac{1}{2}ic)][k_i+\epsilon+(\frac{1}{2}ic)]}$$
$$+\frac{aic(ic+\epsilon-\delta)}{(\epsilon-\delta)[k_i+\delta+(\frac{1}{2}ic)]}+\frac{bic(ic+\delta-\epsilon)}{(\delta-\epsilon)[k_i+\epsilon+(\frac{1}{2}ic)]}. \quad \text{(B6)}$$

If we substitute (B6) on the left-hand side of (B2), put the explicit k dependence of χ, (2.48), in on the right-hand side and simplify we obtain

$$k_i[a(ic+\epsilon-\delta)-b(ic+\delta-\epsilon)]$$
$$+a(ic+\epsilon-\delta)[\epsilon+(\tfrac{1}{2}ic)]-b(ic+\delta-\epsilon)[\delta+(\tfrac{1}{2}ic)]$$
$$-2ic(\epsilon-\delta)=0. \quad \text{(B7)}$$

Since this must be true for all values of k_i, both the coefficient of the k_i and the constant term must be zero. Manipulation of these two terms yields

$$a(\epsilon-\delta+ic)=2ic, \quad \text{(B8a)}$$

$$b(\delta-\epsilon+ic)=2ic. \quad \text{(B8b)}$$

If in (2.36) we let $x=-\delta+\frac{1}{2}(ic)$, we find

$$1-a=\prod_{j=1}^{N}\frac{[k_j+\delta+(\frac{1}{2}ic)]}{k_j+\delta-(\frac{1}{2}ic)}. \quad \text{(B9)}$$

Thus, from (B8a) and (B9) we obtain

$$\prod_{j=1}^{N}\frac{[k_j+\delta+(\frac{1}{2}ic)]}{[k_j+\delta-(\frac{1}{2}ic)]}=\frac{\epsilon-\delta-ic}{\epsilon-\delta+ic}. \quad \text{(B10a)}$$

From (B8) it follows that (B10) must also be true if ϵ and δ are interchanged. Thus,

$$\prod_{j=1}^{N}\frac{[k_j+\epsilon+(\frac{1}{2}ic)]}{[k_j+\epsilon-(\frac{1}{2}ic)]}=\frac{\delta-\epsilon-ic}{\delta-\epsilon+ic}. \quad \text{(B10b)}$$

The condition that β be a null vector can be shown not to contain any new information.

Note added in proof. After this work was completed, a letter by M. Gaudin[9] appeared in Physics Letters in which he presented the results of his independent investigation of this problem. His work gives the generalization of the essential results of this paper, Eqs. (1.25) and (1.26), to the case for an arbitrary number of spin deviates. None of the details of the solution were given.

[9] M. Gaudin, Phys. Letters 24A, 55 (1967).

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ABSENCE OF MOTT TRANSITION IN AN EXACT SOLUTION OF THE SHORT-RANGE, ONE-BAND MODEL IN ONE DIMENSION

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The short-range, one-band model for electron correlations in a narrow energy band is solved exactly in the one-dimensional case. The ground-state energy, wave function, and the chemical potentials are obtained, and it is found that the ground state exhibits no conductor-insulator transition as the correlation strength is increased.

The correlation effect of electrons in a partially filled energy band has been a subject of interest for many years.[1-4] A realistic model which takes this correlation into consideration, and which is hopefully amenable to mathematical treatment, is the short-range, one-band model considered by a number of authors.[2-5] In this model, one pictures the electrons in a narrow energy band hopping between the Wannier states of neighboring lattice sites, with a repulsive interaction energy between two electrons of opposite spins occupying the same lattice site. The central problems of interest have been (a) the possible existence of a "Mott transition" between conducting and insulating states as the strength of the interaction is increased, and (b) the magnetic nature (ferromagnetic or antiferromagnetic) of the ground state. While previous treatments of this model have always been approximate, we have succeeded in solving the model exactly in the one-dimensional case. Our exact result shows that the Mott transition does not occur in the ground state of the one-dimensional model. Furthermore, a general theorem of Lieb and Mattis[6] on one-dimensional systems tells us that the ground state is necessarily antiferromagnetic.

It may be argued that the absence of a Mott transition in one dimension is irrelevant for the study of real three-dimensional systems because of the folkloristic dictum that there are never any phase transitions in one dimension with short-range interactions. In actual fact, the dictum is only true for nonzero temperature; the ground state is another matter. Generally speaking, when a Hamiltonian is considered to be a function of some parameter, U (which in our case is the electron-electron repulsion), singularities with respect to U usually do appear in the ground-state wave function, energy, polarizability, etc., even in one dimension. A good example of this is the one-dimensional Heisenberg chain (to which the present model is very close) which, when considered as a function of the anisotropy parameter, does have two singularities in the ground state and, presumably, no singularities for nonzero temperatures.[7,8]

Consider a crystal (one-, two-, or three-dimensional) of N_a lattice sites with a total of $N \leq 2N_a$ electrons. We suppose that the electrons can hop between the Wannier states of neighboring lattice sites, and that each site is capable of accommodating two electrons of opposite spins, with an interaction energy $U>0$. The Hamiltonian to consider is then[2-5]

$$H = T\sum_{\langle ij\rangle}\sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U\sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^{\dagger}, c_{i\sigma}$ are, respectively, the creation and annihilation operators for an electron of spin σ in the Wannier state at the ith lattice site, and the sum

$$\sum_{\langle ij\rangle}$$

is restricted to nearest-neighbor sites.

First of all, it can be shown that the energy spectrum of H is invariant under the replacement of T by $-T$.[9] Therefore, for simplicity we shall take, in appropriate units, $T=-1$. Since the numbers M of down-spin electrons and M' of up-spin electrons are good quantum numbers ($M+M'=N$), we may designate the ground-state energy of H by $E(M,M';U)$. It is then easy to derive the following relations [by considering holes instead of particles in (1)]:

$$\begin{aligned} E(M,M';U) &= -(N_a - M - M')U \\ &\quad + E(N_a - M, N_a - M'; U) \\ &= MU + E(M, N_a - M'; -U) \\ &= M'U + E(N_a - M, M'; -U). \end{aligned} \quad (2)$$

Without loss of generality, therefore, we may take

$$S_z \equiv \tfrac{1}{2}(N-2M) \geq 0 \text{ and } N \leq N_a$$

(less than half-filled band).

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It can similarly be shown that the maximum energy $G(M,M';U)$ is related to the ground-state energy by

$$G(M,M';U)=M'U-E(N_a-M,M';U).$$

Therefore, a knowledge of the ground-state energies also tells us about the maximum energies.

For a one-dimensional system, the lattice sites can be numbered consecutively from 1 to N_a. Let $f(x_1,x_2,\cdots,x_M,x_{M+1},\cdots,x_N)$ represent the amplitude in ψ for which the down spins are at the sites $x_1,\cdots,x_M$, and the up spins at $x_{M+1},\cdots,x_N$. Then the eigenvalue equation $H\psi=E\psi$ leads to

$$-\sum_{i=1}^{N}\sum_{s=\pm 1} f(x_1,\cdots,x_i+s,\cdots,x_N)$$
$$+U\sum_{i<j}\delta(x_i-x_j)f(x_1\cdots x_N)$$
$$=Ef(x_1\cdots x_N), \tag{3}$$

where it is understood that we require a solution of the form

$$f(x_1,x_2,\cdots,x_M|x_{M+1},x_{M+2},\cdots,x_N) \tag{4}$$

which is antisymmetric in the first M and the last $N-M$ variables.

In each region defined by $1\leq x_{Q1}\leq x_{Q2}\leq\cdots x_{QN}\leq N$, we make the following Ansatz for f:

$$f(x_1,\cdots,x_M|x_{M+1},\cdots,x_N)$$
$$=\sum_P [Q,P]\exp(i\sum_{j=1}^{N} k_{Pj}x_{Qj}), \tag{5}$$

where $P=(P1,P2,\cdots,PN)$ and $Q=(Q1,Q2,\cdots,QN)$ are two permutations of the numbers $(1,2,\cdots,N)$, $\{k_1,k_2,\cdots k_N\}$ is a set of N unequal real numbers, and $[Q,P]$ is a set of $N!\times N!$ coefficients to be determined.

The coefficients $[Q,P]$ are not all independent. The condition of single valuedness (or continuity) of f and the requirement that (5) be a solution of (3) lead to the following:

$$E=-2\sum_{j=1}^{N}\cos k_j \tag{6}$$

and, for all Q and P, the coefficients $[Q,P]$ must be chosen to satisfy the relations

$$[Q,P]=Y_{nm}^{\ ab}[Q,P']. \tag{7}$$

In (7), $Y_{nm}^{\ ab}$ is an operator defined by

$$Y_{nm}^{\ ab}=\frac{-\frac{1}{2}iU}{\sin k_n-\sin k_m+\frac{1}{2}iU}$$
$$+\frac{\sin k_n-\sin k_m}{\sin k_n-\sin k_m+\frac{1}{2}iU}P^{ab}, \tag{8}$$

where, for $j=i+1$,

$$Qi=a=Q'j,\quad Qj=b=Q'i,$$

$$Qk=Q'k \text{ for all } k\neq i,j;$$

$$Pi=m=P'j,\quad Pj=n=P'i,$$

$$Pk=P'k \text{ for all } k\neq i,j;$$

and P^{ab} is an operator which exchanges $Qi=a$ and $Qj=b$.

It is fortunate that the Ansatz (5) and the algebraic consistency conditions (7) and (8) have, in essence, appeared before in the study of the one-dimensional delta-function gas for particles in a continuum. The first solution of that problem was for bosons (symmetric f) by Lieb and Liniger[10] but this case is not relevant here, besides which the consistency conditions there are trivial to solve. The two-component fermion case was solved by McGuire[11] for $M=1$, but again (7) is trivial because of translational invariance. The next development was the solution of the case $M=2$ by Flicker and Lieb[12] by an inelegant algebraic method which could not be easily generalized. However, the case $M=2$ is the simplest one which displays the full difficulty of the problem. Shortly thereafter, Gaudin[13] published the solution of the general-M problem. The method of his brilliant solution did not appear for some time and is now available as his thesis.[14] In the meantime, Yang[15] also discovered the method of solution (essentially the same as Gaudin's) and published it with considerable detail. Here, we have followed Yang's notation with slight modification.

The important point is that our Eqs. (7) and (8) are the same as for the continuum gas except for the replacement of k by $\sin k$ in the latter. This has no effect on the beautiful algebraic analysis which finally leads to the following condi-

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tions which determine the set $\{k_1, k_2, \cdots, k_N\}$:

$$N_a k_j = 2\pi I_j + \sum_{\beta=1}^{M} \theta(2\sin k_j - 2\Lambda_\beta), \quad j = 1, 2, \cdots, N, \tag{9}$$

where the Λ's are a set of real numbers related to the k's through

$$-\sum_{j=1}^{N} \theta(2\Lambda_\alpha - 2\sin k_j) = 2\pi J_\alpha - \sum_{\beta=1}^{M} \theta(\Lambda_\alpha - \Lambda_\beta), \quad \alpha = 1, 2, \cdots, M, \tag{10}$$

$$\theta(p) \equiv -2\tan^{-1}(2p/U), \quad -\pi \leq \theta < \pi, \tag{11}$$

and I_j = integers (or half-odd integers) for M = even (or odd), J_α = integers (or half-odd integers) for M' = odd (or even). An immediate consequence is

$$\sum_{j=1}^{N} k_j = \frac{1}{N_a}\left(\sum_j I_j + \sum_\alpha J_\alpha\right). \tag{12}$$

For the ground state, J_α and I_j are consecutive integers (or half-odd integers) centered around the origin and satisfying $\sum_j k_j = 0$.

In the limit of $N \to \infty$, $N_a \to \infty$, $M \to \infty$ with the ratios N/N_a, M/N_a kept finite, the real numbers k and Λ are distributed continuously between $-Q$ and $Q \leq \pi$ and $-B$ and $B \leq \infty$, with density functions $\rho(k)$ and $\sigma(\Lambda)$, respectively. Equations (9) and (10) then lead to the coupled integral equations for the distribution function $\rho(k)$ and $\sigma(\Lambda)$:

$$2\pi\rho(k) = 1 + \cos k \int_{-B}^{B} \frac{8U\sigma(\Lambda)d\Lambda}{U^2 + 16(\sin k - \Lambda)^2}, \tag{13}$$

$$\int_{-Q}^{Q} \frac{8U\rho(k)dk}{U^2 + 16(\Lambda - \sin k)^2} = 2\pi\sigma(\Lambda) + \int_{-B}^{B} \frac{4U\sigma(\Lambda')d\Lambda'}{U^2 + 4(\Lambda - \Lambda')^2}, \tag{14}$$

where Q and B are determined by the conditions

$$\int_{-Q}^{Q} \rho(k)dk = N/N_a, \tag{15}$$

$$\int_{-B}^{B} \sigma(\Lambda)d\Lambda = M/N_a. \tag{16}$$

The ground-state energy (6) now becomes

$$E = -2N_a \int_{-Q}^{Q} \rho(k)\cos k dk. \tag{17}$$

We have established the following:

(a) Equations (13)-(16) have a unique solution which is positive for all allowed B and Q.

(b) M/N is a monotonically increasing function of B reaching a maximum of $\frac{1}{2}$ at $B = \infty$. This is the antiferromagnetic case, $S_z = 0$, and corresponds to the absolute ground state.

(c) N/N_a is a monotonically increasing function of Q, reaching a maximum of 1 (half-filled band) at $Q = \pi$.

For $B = \infty$ and $Q = \pi$, (13)-(16) can be solved in closed form by Fourier transforms with the result

$$\sigma(\Lambda) = (2\pi)^{-1} \int_0^\infty \operatorname{sech}(\tfrac{1}{4}\omega U) \times \cos(\omega\Lambda) J_0(\omega) d\omega, \tag{18}$$

$$\rho(k) = (2\pi)^{-1} + \pi^{-1}\cos k \times \int_0^\infty \frac{\cos(\omega \sin k) J_0(\omega) d\omega}{1 + \exp(\frac{1}{2}\omega U)}, \tag{19}$$

$$E \equiv E(\tfrac{1}{2}N_a, \tfrac{1}{2}N_a; U) = -4N_a \int_0^\infty \frac{J_0(\omega)J_1(\omega)d\omega}{\omega[1 + \exp(\frac{1}{2}\omega U)]}, \tag{20}$$

where J_0 and J_1 are Bessel functions.

To investigate whether the ground state is conducting or insulating, we compute the chemical

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potentials μ_+ and μ_- as defined in a forthcoming paper by Mattis[16]:

$$\mu_+ \equiv E(M+1,M;U)-E(M,M;U),$$
$$\mu_- \equiv E(M,M;U)-E(M-1,M;U). \quad (21)$$

If μ_+ and μ_- are equal, the system has the property of a conductor. If, on the other hand, we find $\mu_+ > \mu_-$, then the system shares the property of an insulator. We can compute μ_- directly from (9) and (10) by replacing $M \to M-1$ and $N \to N-1$, while letting all the k's, Λ's, and their distribution functions change slightly. The procedure is quite similar to the calculation of the excitation spectrum of the continuum gas.[10] If $N < \frac{1}{2}N_a$, we can compute μ_+ in the same way and thereby find that $\mu_+ = \mu_-$ for all U. If, however, N is exactly $\frac{1}{2}N_a$, then we must compute μ_+ by using the first line of (2) which tells us that

$$\mu_+ = U - \mu_- \text{ (half-filled band)}. \quad (22)$$

The calculation of μ_- can be done in closed form for a half-filled band with the result

$$\mu_- - 2 = -4\int_0^\infty \frac{J_1(\omega)d\omega}{\omega[1+\exp(\frac{1}{2}\omega U)]}$$
$$= -4\sum_{n=1}^{\infty}(-1)^n[(1+\tfrac{1}{4}n^2U^2)^{\frac{1}{2}}-\tfrac{1}{2}nU]. \quad (23)$$

It can be established from (22) and (23) that, indeed, $\mu_+ > \mu_-$ for $U > 0$, and

$$\lim_{U\to 0} \mu_\pm = 0.$$

Therefore, we conclude that the ground state for a half-filled band is insulating for any nonzero U, and conducting for $U = 0$. That is, there is no Mott transition for nonzero U. This absence of a Mott transition is also reflected by the fact that the ground-state energy and the ground-state wave function are analytic in U on the real axis (except at the origin).

We have also investigated the excitation spectrum $E(p)$ for a given total momentum $\sum_j k_j = p$ and a given value of S_z. Just as in the case of a continuum gas for which the spectrum can be regarded as consisting of several elementary excitations,[10,15] we find three types of excitations: (I) a "hole" state in the Λ distribution, (II) a "hole" state in the k distribution, and (III) a "particle" state in the k distribution. While the $S_z = 0$ spin-wave state may have any of these three types of spectra, the $S_z = 1$ spin-wave state is always associated with the type-I spectrum. The type-I excitation has the lowest energy and is characterized by a double periodicity similar to that of an antiferromagnetic chain.[7] In the limit $U \to 0$, it goes over to $E(p) = |\sin p|$, while the type-II and -III spectra have the identical limiting form $E(p) = |2\sin(\frac{1}{2}p)|$. Detailed discussions of these matters will be given elsewhere.

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$$\exp[i\pi\sum_\sigma\sum_{i\in A} c_{i\sigma}^\dagger c_{i\sigma}]$$

which changes $c_{i\sigma}$ to $-c_{i\sigma}$ and $c_{i\sigma}^\dagger$ to $-c_{i\sigma}^\dagger$ for $i \in A$. This transformation does not change the number operator.

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Part XIV

Luttinger Model

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Exact Solution of a Many-Fermion System and Its Associated Boson Field

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Luttinger's exactly soluble model of a one-dimensional many-fermion system is discussed. We show that he did not solve his model properly because of the paradoxical fact that the density operator commutators $[\rho(p), \rho(-p')]$, which always vanish for any finite number of particles, no longer vanish in the field-theoretic limit of a filled Dirac sea. In fact the operators $\rho(p)$ *define* a boson field which is *ipso facto* associated with the Fermi–Dirac field. We then use this observation to solve the model, and obtain the exact (and now nontrivial) spectrum, free energy, and dielectric constant. This we also extend to more realistic interactions in an Appendix. We calculate the Fermi surface parameter $\tilde{n}_k$, and find: $\partial\tilde{n}_k/\partial k|_{k_F} = \infty$ (i.e., there exists a sharp Fermi surface) only in the case of a sufficiently weak interaction.

I. INTRODUCTION

THE search for a soluble but realistic model in the many-electron problem has been just about as unfruitful as the historic quest for the philosopher's stone, but has equally resulted in valuable byproducts. For example, 15 years ago Tomonaga[1] published a theory of interacting fermions which was soluble only in one dimension with the provision that certain truncations and approximations were introduced into his operators. Nevertheless he had success in showing approximate boson-like behavior of certain collective excitations, which he identified as "phonons." (Today we would denote these as "plasmons," following the work of Bohm and Pines.[2]) Lately, Luttinger[3] has revived interest in the subject by publishing a variant model of spinless and massless one-dimensional interacting fermions, which demonstrated a singularity at the Fermi surface, compatible with the results of the modern many-body perturbation theory.[4]

Unfortunately, in calculating the energies and wavefunctions of his model Hamiltonian, Luttinger fell prey to a subtle paradox inherent in quantum field theory[5] and *therefore did not achieve a correct solution of the problem he himself had posed.* In the present paper we shall give the solution to his interesting problem and calculate the free energy. We shall show the existence of collective plasmon modes, and shall calculate the singularity at the Fermi surface (which may in fact disappear if the interaction is strong enough), the energy of the plasmons, and the (nontrivial) dielectric constant of the system. In an Appendix we shall show how the model may be generalized in such a manner as to remove certain restrictions on the interactions which Luttinger had found necessary to impose.

It is fortunate that solid-state and many-body theorists have so far been spared the plagues of quantum field theory. Second quantization has been often just a convenient bookkeeping arrangement to save us from writing out large determinantal wavefunctions. However there is a difference between very large determinants and *infinitely* large ones; we shall show that one of the important differences *is the failure of certain commutators to vanish* in the field-theoretic limit when common sense and experience based on finite N tells us they *should* vanish! (Here N refers to the number of particles in the field.)

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[5] Luttinger made a transformation, L (8), which was canonical in appearance only. But in the language of G. Barton [*Introduction to Advanced Field Theory*, (Interscience Publishers, Inc., New York, 1963), pp. 126 *et seq.*] this transformation connected two "unitarily inequivalent" Hilbert spaces, which has as a consequence that commutators, among other operators, must be reworked so as to be well-ordered in fermion field operators. It was first observed by Julian Schwinger [Phys. Rev. Letters 3, 296 (1959)] that the very fact that one postulates the existence of a ground state (i.e., the filled Fermi sea) *forces* certain commutators to be nonvanishing even though in first quantization they automatically vanish. The "paradoxical contradictions" of which Schwinger speaks seem to anticipate the difficulties in the Luttinger model.

We shall show that these nonvanishing commutators *define* boson fields which must *ipso facto* always be associated with a Fermi–Dirac field, and we shall use the ensuing commutation relations to solve Luttinger's model exactly. Because this model is soluble both in the Hilbert space of finite N and also in the Hilbert space $N = \infty$, with different physical behavior in each, we believe it has applications to the *theory of fields* which go beyond the study of the many-electron problem. The model can be extended to the case of electrons with spin. This has interesting consequences in the band *theory of ferromagnetism*, as will be discussed in some detail in an article under preparation.[5a]

II. MODEL HAMILTONIAN

We recall Luttinger's Hamiltonian[3] and recapitulate some of his results:

$$H = H_0 + H', \tag{2.1}$$

where the "unperturbed" part is

$$H_0 = \int_0^L dx\ \psi^+(x)\sigma_3 p\psi(x) \tag{2.2a}$$

$$= \sum_k (a_{1k}^* a_{1k} - a_{2k}^* a_{2k})k, \tag{2.2b}$$

and the interaction is

$$H' = 2\lambda \iint_0^L dx\,dy\ \psi_1^+(x)\psi_1(x) \times V(x-y)\psi_2^+(y)\psi_2(y) \tag{2.3a}$$

$$= \frac{2\lambda}{L} \sum \delta_{k_1+k_3,k_2+k_4} v(k_3 - k_4) \times a_{1k_1}^* a_{1k_2} a_{2k_3}^* a_{2k_4}. \tag{2.3b}$$

Here ψ is a two-component field and the form (b) of the operator is obtained from (a) by setting

$$\psi = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \begin{pmatrix} a_{1k} \\ a_{2k} \end{pmatrix}$$

and

$$\psi^+ = \frac{1}{\sqrt{L}} \sum_k e^{-ikx}(a_{1k}^*,\ a_{2k}^*), \tag{2.4}$$

with a_{ik}'s defined to be anticommuting fermion operators which obey the usual relations

$$a_{ik}a_{i'k'} + a_{i'k'}a_{ik} \equiv \{a_{ik},\ a_{i'k'}\} = 0$$
$$\{a_{ik}^*,\ a_{i'k'}^*\} = 0, \text{ and } \{a_{ik},\ a_{i'k'}^*\} = \delta_{ii'}\delta_{kk'}. \tag{2.5}$$

Luttinger noted that for an appropriate operator S_0, the canonical transformation

$$\tilde{H} = e^{i\lambda S_0} H e^{-i\lambda S_0} \tag{2.6}$$

gave the result that

$$\tilde{H} = H_0, \tag{2.7}$$

and consequently that *the spectrum of* $H = H_0 + H'$ *was the same as that of* H_0, *independent of the interaction* $V(x-y)$. This can be explicitly verified for his choice of

$$S_0 = \iint_0^L dx\,dy\ \psi_1^+(x)\psi_1(x)E(x-y)\psi_2^+(y)\psi_2(y), \tag{2.8}$$

where $E(x)$, not to be confused with the energy E, is defined by:

$$\partial E(x-y)/\partial x \equiv V(x-y), \tag{2.9}$$

assuming that

$$\bar{V} \equiv \frac{1}{L}\int_0^L V(x)\,dx = 0. \tag{2.10}$$

In the Appendix we shall show among other things how to generalize to $\bar{V} \neq 0$. It is also simple and instructive to verify Eqs. (2.6) and (2.7) somewhat differently by using the *first* quantization,

$$H_0 = -i\sum_{n=1}^N \frac{\partial}{\partial x_n} + i\sum_{m=1}^M \frac{\partial}{\partial y_m} \tag{2.11}$$

and

$$H' = 2\lambda \sum_{n=1}^N \sum_{m=1}^M V(x_n - y_m), \tag{2.12}$$

where N and M are, respectively, the total number of "1" particles and "2" particles, with coordinates x_n and y_m, respectively. The properly antisymmetrized wavefunctions are given by

$$\Psi = \det|e^{ik_i x_j}|\ \det|e^{iq_i y_j}| \times \exp\left\{\sum_{n=1}^N \sum_{m=1}^M i\,E(x_n - y_m)\right\}. \tag{2.13}$$

Using Eqs. (2.9) and (2.10), Ψ is readily seen to obey Schrödinger's equation

$$H\Psi = E\Psi \tag{2.14}$$

with just the unperturbed eigenvalue

$$E = \sum_{n=1}^N k_n - \sum_{m=1}^M q_m. \tag{2.15}$$

The wavenumbers are of the form

$$k_i \quad \text{or} \quad q_i = 2\pi \text{ integer}/L, \tag{2.16}$$

as required for periodic boundary conditions. This is in exact agreement with the results of Ref. 3, and can also be checked in perturbation theory; first-

[5a] D. Mattis, Physics 1, 184 (1964).

order perturbation theory also gives vanishing results, and indeed, it is easy to verify that to every order in λ the cancellation is complete, in accordance with the exact result given above.

Up to this point, Luttinger's analysis (which we have briefly summarized) is perfectly correct. It is the next step that leads to difficulty. The Hamiltonian discussed so far has no ground-state energy; in order to remove this obstacle, and thereby establish contact with a real electron gas, Luttinger proposed modifying the model by "filling the infinite sea" of negative energy levels (i.e., all states with $k_1 <$ and $q_2 > 0$). Following L(8) we define b's and c's obeying the usual anticommutators, such that

$$a_{1k} = \begin{cases} b_k & k \geq 0 \\ c^*_{\ k} & k < 0, \end{cases}$$

and (2.17)

$$a_{2k} = \begin{cases} b_k & k < 0 \\ c^*_k & k \geq 0. \end{cases}$$

Using this notation the total particle-number operator becomes

$$\mathfrak{N} = \sum_{\alpha 1 1 k} b^+_k b_k - c^+_k c_k \tag{2.17a}$$

(i.e., the number of particles minus the number of holes).

Since the Hamiltonian commutes with $\mathfrak{N}$ we can demand that $\mathfrak{N}$ have eigenvalue N_0. In the noninteracting ground state there are no holes and the b particles are filled from $-k_F$ to k_F where $k_F = \pi(N_0/L) = \pi\rho$. The noninteracting ground-state energy is $N_0\pi\rho +$ energy of the filled sea (W).

The kinetic energy assumes the form

$$H_0 = \sum_{\alpha 1 1 k} (b^*_k b_k + c^*_k c_k)\,|k| + W, \tag{2.18}$$

where

$$W = (\sum_{k<0} k - \sum_{k>0} k) \tag{2.18a}$$

is the infinite energy of the filled sea, an uninteresting c number which we drop henceforth in accordance with Luttinger's prescription. The interaction [H', Eq. (2.3) and the operator S_0, Eq. (2.8)] can also be expressed in the new language by means of the substitution (2.17). The reader will no doubt be surprised, as indeed we were, to find that now with the new operators, *Eq.* (2.7), *with $\tilde{H}$ defined in* (2.6), *is no longer obeyed.*

Upon further reflection one sees that this must be so, on the basis of very general arguments. In the new Hilbert space defined by the transformation to the particle–hole language (2.17), H is no longer unbounded from below and now has a ground state.

A general and inescapable *concavity theorem* states that if $E_0(\lambda)$ is the ground-state energy in the presence of interactions, (2.3), then

$$\partial^2 E_0(\lambda)/\partial\lambda^2 < 0. \tag{2.19}$$

This inequality is incompatible with the previous result, viz. all E = independent of λ, which was possible only in the strange case of a system without a ground state.

The same thing can be seen more trivially using second-order perturbation theory (first-order perturbation theory vanishes). It is easily seen that

$$E_0^{(2)} = -\left(\frac{2\lambda}{L}\right)^2 \sum_k \frac{|v(k)|^2}{2k} n_1(k) n_2(-k), \tag{2.20}$$

where $n_1(k)$ and $n_2(k)$ are the number of ways of shifting a particle of type "1" and type "2" respectively by an amount k to an unoccupied state. A simple geometric exercise will convince the reader of the following facts: (1) if we start with a state having a finite number of particles, then n_1 and n_2 are *always* even functions of k (i.e., there are just as many ways to increase the momentum by k as to decrease it by the same amount.) (2) If we start with a filled infinite sea then there is no way to decrease the momentum of the "1" particles nor to increase the momentum of "2" particles. Hence for this second case $n_1(k)n_2(-k)$ is nonzero only for $k > 0$. Thus $E_0^{(2)}$ vanishes for a state with a finite number of particles, but it is negative for a filled sea.

If the reader is unconvinced by perturbation theory, then he can easily prove that E_0 is lowered by doing a variational calculation.

What has gone wrong? We turn to some algebra to resolve this paradox, and following this, present a solution of the field-theoretic problem defined by $H_0 + H'$ in the representation of b's and c's.

III. CASE OF THE FILLED DIRAC SEA

The various relevant operators are given below; the form (a) of each equation will *not* be used in the bulk of the paper, and is just given here for completeness. In the following equations, $p > 0$.

$$\rho_1(+p) \equiv \sum_k a^*_{1\,k+p} a_{1\,k} \tag{3.1a}$$

$$= \sum_{k<-p} c_{k+p} c^*_k + \sum_{-p\leq k<0} b^*_{k+p} c^*_k + \sum_{k\geq 0} b^*_{k+p} b_k, \tag{3.1b}$$

$$\rho_1(-p) \equiv \sum_k a^*_{1k} a_{1\,k+p} \tag{3.2a}$$

$$= \sum_{k<-p} c_k c^*_{k+p} + \sum_{-p\leq k<0} c_k b_{k+p} + \sum_{k\geq 0} b^*_k b_{k+p}, \tag{3.2b}$$

$$\rho_2(+p) \equiv \sum_k a_{2\,k+p}^* a_{2\,k} \tag{3.3a}$$

$$= \sum_{k<-p} b_{k+p}^* b_k + \sum_{-p\le k<0} o_{k+p} b_k + \sum_{k\ge 0} o_{k+p} c_k^*, \tag{3.3b}$$

$$\rho_2(-p) \equiv \sum_k a_{2\,k}^* a_{2\,k+p} \tag{3.4a}$$

$$= \sum_{k<-p} b_k^* b_{k+p} + \sum_{-p\le k<0} b_k^* c_{k+p}^* + \sum_{k>0} o_k c_{k+p}^*. \tag{3.4b}$$

Equations (3.1a)–(3.4a) give the density operators in the original representation, so let us calculate in this language a commutator such as (assume $p \geq p' \geq 0$ for definiteness)

$$[\rho_1(-p),\ \rho_1(p')] = \sum_{k,k'} [a_{1\,k}^* a_{1\,k+p},\ a_{1\,k'+p'}^* a_{1\,k'}]$$

$$= \sum_{k=-\infty}^{+\infty} a_{1\,k}^* a_{1\,k+p-p'} - \sum_{k=-\infty}^{+\infty} a_{1\,k+p'}^* a_{1\,k+p} = 0. \tag{3.5}$$

The zero result could have been expected by writing the operators in first quantization:

$$\rho_1(-p) = \sum_n e^{-ipx_n} \quad \text{and} \quad \rho_2(p) = \sum_m e^{ipy_m}, \tag{3.6}$$

whence they evidently commute. Nevertheless, the zero result is achieved in (3.5) only through the almost "accidental" cancellation of two operators, each of which may diverge in the field-theory limit when $N = \infty$. We now show that in that limit the operators in fact no longer cancel, by evaluating the commutator using form (b) for the density operators. It is a matter of only some minor manipulation to obtain the important new result:

$$[\rho_1(-p),\ \rho_1(p')] = [\rho_2(p),\ \rho_2(-p')]$$

$$= \delta_{p,p'} \sum_{-p<k<0} 1 = \frac{pL}{2\pi}\,\delta_{p,p'}, \quad (p' > 0). \tag{3.7a}$$

In addition,

$$[\rho_1(p),\ \rho_2(p')] = 0. \tag{3.7b}$$

A quick check is provided by evaluating the vacuum expectation value

$$\langle 0|\ [\rho_1(-p),\ \rho_1(p)]\ |0\rangle$$

$$= \sum_{-p<k,k'<0} \langle 0|\ o_k b_{k+p} b_{k'+p}^* o_{k'}^*\ |0\rangle = pL/2\pi, \tag{3.8}$$

which is exactly what is expected on the basis of the previous equation. Evidently the form (b) of the operators $(2\pi/pL)^{+\frac{1}{2}}\rho_1(+p)$ and $(2\pi/pL)^{+\frac{1}{2}}\rho_2(-p)$ have properties of boson raising operators [call them $A^*(p)$ and $B^*(-p)$] and $(2\pi/pL)^{+\frac{1}{2}}\rho_1(-p)$ and $(2\pi/pL)^{+\frac{1}{2}}\rho_2(+p)$ have properties of boson lowering operators [$A(p)$ and $B(-p)$], i.e.,

$$[A, B] = [A^*, B] = 0,$$
$$[A(p),\ A^*(p')] = [B(-p),\ B^*(-p)] = \delta_{p,p'}. \tag{3.9}$$

The B field is the continuation of the A field to negative p; therefore together they form a *single* boson field defined for all p.

The relationship of the $\rho(p)$'s to Luttinger's $N(x)$'s, L(25), is obtained by using (2.4):

$$N_1(x) = \psi_1^*(x)\psi_1(x) = \frac{1}{L}\sum_p \rho_1(p)e^{-ipx},$$
$$N_2(x) = \psi_2^*(x)\psi_2(x) = \frac{1}{L}\sum_p \rho_2(p)e^{-ipx}. \tag{3.10}$$

IV. SOLUTIONS OF THE MODEL HAMILTONIAN

Before making use of the results of the previous section, we remark that $\rho_1(+p)$ and $\rho_2(-p)$ are exact raising operators of H_0, and $\rho_1(-p)$ and $\rho_2(p)$ are exact lowering operators of H_0 corresponding to excitation energies p. That is,

$$[H_0,\ \rho_1(\pm p)] = \pm p\rho_1(\pm p),$$
$$[H_0,\ \rho_2(\pm p)] = \mp p\rho_2(\pm p). \tag{4.1}$$

The identification of the ρ's with boson operators made in the previous section suggested to us the possibility of constructing a new operator T which obeys the same equations (4.1), as H_0. This is indeed possible, if we define T as follows:

$$T \equiv \frac{2\pi}{L}\sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\} \tag{4.2}$$

[the ρ's being defined here and in the remainder of the paper by Eqs. (3.1b)—(3.4b), i.e., always in the hole-particle representation]. It follows that

$$[T,\ \rho_1(\pm p)] = \pm p\rho_1(\pm p) \tag{4.3}$$

as required, and similarly for $\rho_2(\mp p)$. Therefore, let us decompose H into two parts

$$H = H_1 + H_2 \tag{4.4}$$

with

$$H_1 = H_0 - T = \Big\{\sum_k |k|\ (b_k^* b_k + o_k^* c_k)$$
$$- \frac{2\pi}{L}\sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\}\Big\}, \tag{4.5}$$

and

$$H_2 = H' + T$$
$$= \frac{1}{L}\Big[2\lambda \sum_{p>0} \{v(p)\rho_1(-p)\rho_2(p) + v(-p)\rho_1(p)\rho_2(-p)\}$$
$$+ 2\pi \sum_{p>0} \{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\}\Big] \tag{4.6}$$

with $v(p)$ = real, even function of p. By actual construction, all the ρ operators which appear in H_2

commute with H_1. This will be an important feature in constructing an exact solution of the model. We define an Hermitian operator S,

$$S = \frac{2\pi i}{L} \sum_{\text{all } p} \frac{\varphi(p)}{p} \rho_1(p)\rho_2(-p), \tag{4.7}$$

where $\varphi(p)$ is also a real, even, function of p to be determined subsequently by imposing a condition that the unitary transformation e^{iS} diagonalize H_2. First we evaluate the effect of such a transformation on various operators. It commutes with H_1,

$$e^{iS}H_1e^{-iS} = H_1 = H_0 - T, \tag{4.8}$$

because both ρ_1 and ρ_2 appearing in S commute with H_1, as noted above. In the following, p can have either sign:

$$e^{iS}\rho_1(p)e^{-iS} = \rho_1(p)\cosh\varphi(p) + \rho_2(p)\sinh\varphi(p), \tag{4.9}$$

$$e^{iS}\rho_2(p)e^{-iS} = \rho_2(p)\cosh\varphi(p) + \rho_1(p)\sinh\varphi(p). \tag{4.10}$$

We have verified that this transformation is a proper unitary transformation and preserves commutation relations (3.7) as well as anticommutation relations (2.5), and the reader may easily check this point. H_2 is brought into canonical form by requiring that in (exp iS) H_2 (exp $-iS$) there be no cross terms such as $\rho_1(p)\rho_2(-p)$. This leads to the equation

$$\tanh 2\varphi = -\lambda v(p)/\pi, \tag{4.11}$$

which cannot be obeyed unless

$$|\lambda v(p)| < \pi \quad \text{for all} \quad p. \tag{4.12}$$

Equation (4.12) serves to limit the magnitude of potentials capable of having well-behaved solutions (e.g., a real ground-state energy). For the more realistic potentials discussed in the Appendix, there is also a more realistic bound on $v(p)$: there, $v(p)$ may not be *too* attractive, but it can have any magnitude when it is repulsive, i.e., positive.

With the choice of φ in (4.11), the evaluation of H_2 becomes

$$e^{iS}H_2e^{-iS} = \frac{2\pi}{L} \sum_{p>0} \operatorname{sech} 2\varphi(p)\{\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)\} - \sum_{p>0} p(1 - \operatorname{sech} 2\varphi). \tag{4.13a}$$

The second term is the vacuum renormalization energy

$$W_1 = -\sum_{p>0} p(1 - \operatorname{sech} 2\varphi) = \frac{L}{2\pi}\int_0^\infty dp\, p\left\{\left(1 - \frac{\lambda^2 v^2(p)}{\pi^2}\right)^{\frac{1}{2}} - 1\right\}. \tag{4.13b}$$

It may be expanded in powers of λ to effect a comparison with Goldstone's many-body perturbation theory[4]; we have checked that they agree to third order.

The problem is now formally solved, for we can find all the eigenfunctions and eigenvalues by studying Eqs. (4.4), (4.8), and (4.13). First notice that the operator T does not depend upon the interaction and that if there is *no interaction* we could write the Hamiltonian either as

$$H = H_0, \tag{4.14a}$$

or as

$$H = (H_0 - T) + T = H_1 + H_2. \tag{4.14b}$$

Since H_1 and H_2 commute, every eigenstate, Ψ, of H may be assumed to be an eigenfunction of H_1 and H_2 separately. Moreover, Ψ may also be assumed to be an eigenfunction of each $\alpha_p = A_p^+A_p$ and $\beta_p = B_{-p}^+B_{-p}$ for all $p > 0$, since these operators commute with H and $\mathfrak{N}$.

Evidently (4.14a) and (4.14b) provide two different ways of viewing the noninteracting spectrum. H_0 is quite degenerate: the raising operators of H_0 are the b^+'s and c^+'s. By requiring that Ψ also be an eigenstate of α_p, β_p and H, we are merely attaching quantum numbers to the degenerate levels of H_0. If $\alpha_p\Psi = n_p\Psi$ and $\beta_p\Psi = m_p\Psi$ (where n_p and m_p are of course integers), we say that we have n_p plasmons of momentum p and m_p plasmons of momentum $-p$. With no interaction the energy of a plasmon is

$$\epsilon(p) = |p|. \tag{4.15}$$

We may speak of H_1 as the quasiparticle part of the Hamiltonian; in H_1 the operator T plays the role of subtracting the plasmon part of the energy from H_0.

When we turn on the interaction, the above description of the energy levels is still valid, except that now we are *forced* to use the form (4.14b) because H_2 is no longer T. The degeneracy of H is partially removed by the interaction, because now the energy of a plasmon is

$$\epsilon'(p) = |p| \operatorname{sech} 2\varphi(p). \tag{4.16}$$

Notice that the plasmon energy is always *lowered* [and therefore the plasmons cannot propagate faster than the speed of light $c = 1$, i.e., $d\epsilon'/dp \leq 1$. In the more realistic case discussed in the Appendix, the plasmon energy *can* be increased by the interaction although $d\epsilon'/dp \leq 1$ is always obeyed.] by the interaction; if (4.12) is violated the plasmon energy is no longer real and the system becomes unstable. Note, there are no plasmons in the ground state, so that W_1 (4.13), is the shift in the ground-state energy of the system.

There is one important point, however, that requires some elucidation. We would like to be able to say that in view of the fact that H_1, $\alpha(p)$, and $\beta(p)$

conserve particle number, the most general energy level of H (fixed N_0) is the sum of *any* energy of H_1 (same N_0, and no plasmons) plus *any* (plasmon) energy of H_2 (note: the plasmon spectrum is independent of N_0). Were we dealing with a finite-dimensional vector space, such a statement would not be true, for even though H_1 and H_2 commute they could not possibly be independent. Thus, if H_2 had n eigenvalues $e_1, \cdots, e_n$, and if H_1 had an equal number $E_1, \cdots, E_n$ the general total eigenvalue would not be *any* combination of $e_i + E_i$ for this would give too many values (viz. n^2 instead of n.) But we are dealing with an infinite-dimensional Hilbert space and the additivity hypothesis is in fact true for the present model.

To prove this assertion we consider any eigenstate Ψ which is necessarily parameterized by the integers n_p and m_p. Consider the state $\Phi = \{\prod_p (A_p)^{n_p}(B_p)^{m_p}\}\Psi$. The state Φ is nonvanishing and has quantum numbers $n_p = 0 = m_p$. It is also an eigenstate of H_1 with energy $E_1(\Psi)$. In addition (and this is the important point) the state Ψ may be recovered from Φ by the equation

$$\Psi = \text{const} \times \{\prod_p (A_p^+)^{n_p}(B_p^+)^{m_p}\}\Phi.$$

To every state Ψ, therefore, there corresponds a *unique* state Φ from which it may be obtained using raising operators. Conversely, to any eigenstate of H_1 (for fixed N_0) we may apply raising operators as often as we please and obtain a new (nonvanishing) eigenstate. Thus the general energy is an arbitrary sum of quasiparticle and plasmon energies.

It may be wondered where we used the fact that the Hilbert space is infinite-dimensional in the above proof. The answer lies in the boson commutation relations of the A's and B's. It is impossible to have such relations in a finite-dimensional vector space.

The eigenvalues corresponding to these states Φ will be labeled in some order, E_i $(i = 1, 2, \cdots)$, so that the total canonical partition function $Z(\lambda)$ and the free energy $F(\lambda)$ are given by

$$Z(\lambda) = e^{-F(\lambda)/kT} = (\sum_i e^{-E_i/kT})(e^{-W_1/kT}) \prod_{\substack{\text{all } p \\ \neq 0}} \left(\sum_{n=0}^{\infty} e^{-n\epsilon'(p)/kT}\right). \tag{4.17}$$

The first factor is difficult to evaluate directly. However it can be obtained circuitously by noting that the energies E_i are independent of λ and therefore

$$Z(0) = e^{-F(0)/kT} = (\sum_i e^{-E_i/kT}) \prod_{\substack{\text{all } p \\ \neq 0}} \left(\sum_{n=0}^{\infty} e^{-n\epsilon(p)/kT}\right). \tag{4.18}$$

But the second factor can be trivially evaluated, as can $F(0)$ = free energy of noninteracting fermions. Therefore we use (4.18) to eliminate the trace involving the E_i's in (4.17), with the final result:

$$F(\lambda) = F(0) + W_1 + 2kT \sum_{p>0} \ln \{(1 - e^{-\epsilon'(p)/kT})/(1 - e^{-\epsilon(p)/kT})\}, \tag{4.19}$$

where ϵ and ϵ' are given in (4.15) and (4.16). It is noteworthy that the ground state and free energy both diverge in the case of a δ-function potential.

V. EVALUATION OF THE MOMENTUM DISTRIBUTION

In this section we calculate the mean number of particles with momentum k. This quantity is $\bar{n}_k$ and is the expectation value of

$$n_k = b_k^+ b_k \tag{5.1}$$

in the ground state. Since $\bar{n}_k$ is an even function of k we need only consider $k > 0$, and it is further convenient to introduce a Fourier transform so that [using (2.4)]

$$\bar{n}_k = \frac{1}{L} \int_0^L\int ds\, dt\, e^{ik(s-t)} I(s, t). \tag{5.2}$$

Here

$$I(s, t) = \langle\Psi|\, \psi_1^+(s)\psi_1(t)\, |\Psi\rangle = \langle\Psi_0|\, e^{iS}\psi_1^+(s)e^{-iS}e^{iS}\psi_1(t)e^{-iS}\, |\Psi_0\rangle, \tag{5.3}$$

where S is given by (4.7), Ψ is the new ground state, and Ψ_0 is the noninteracting ground state which is filled with b particles between $-k_F$ and k_F and has no holes (or c particles). This assignment depends on there having been no level crossing, which can be readily verified using (4.7)–(4.13).

In order to calculate the quantity $e^{iS}\psi_1(t)e^{-iS}$ we introduce the auxiliary operator

$$f_\sigma(t) = e^{i\sigma S}\psi_1(t)e^{-i\sigma S}, \tag{5.4}$$

where σ is a c number. We observe that $f_1(t)$ is the desired quantity while

$$f_0(t) = \psi_1(t). \tag{5.5}$$

In addition,

$$\partial f/\partial\sigma = e^{i\sigma S} i[S, \psi_1(t)]e^{-i\sigma S} = e^{i\sigma S}[2\pi/L \sum_p \rho_2(-p)\varphi(p)p^{-1}e^{ipt}]e^{-i\sigma S} f_\sigma(t), \tag{5.6}$$

where we have used the commutation relations (3.7) as well as the fact that ψ_1 commutes with ρ_2. Equa-

tion (5.6) is a differential equation for $f_\sigma(t)$ and (5.5) is the boundary condition. The solution is

$$f_\sigma(t) = W_\sigma(t)R_\sigma(t)\psi_1(t), \tag{5.7}$$

where

$$W_\sigma(t) = \exp\{2\pi/L \sum_{p>0} [\rho_1(-p)e^{ipt} - \rho_1(p)e^{-ipt}]p^{-1}[\cosh \sigma\varphi(p) - 1]\} \tag{5.8}$$

and

$$R_\sigma(t) = \exp\{2\pi/L \sum_{p>0} [\rho_2(-p)e^{ipt} - \rho_2(p)e^{-ipt}]p^{-1} \sinh \sigma\varphi(p)\} \tag{5.9}$$

The reader may verify that (5.7) satisfies (5.5) and (5.6) by using the commutation relations (3.7). We recall the well-known rule that

$$\exp(A + B) = \exp(A) \exp(B) \exp(-1/2[A, B]) \tag{5.10}$$

when $[A, B]$ commutes with A and B. From here on we shall set $\sigma = 1$ and drop it as a subscript. We note that since $\rho_1(p)^+ = \rho_1(-p)$ and $\rho_2(p)^+ = \rho_2(-p)$,

$$R^+(t) = R^{-1}(t) \quad \text{and} \quad W^+(t) = W^{-1}(t). \tag{5.11}$$

We also note that R and W commute with each other. Thus, (5.3) becomes

$$I(s, t) = \langle\Psi_0| \psi_1^+(s)R^{-1}(s)W^{-1}(s)W(t)R(t)\psi_1(t) |\Psi_0\rangle = I_1(s, t)I_2(s, t), \tag{5.12}$$

where

$$I_1(s, t) = \langle\Psi_1| \psi_1^+(s)W^{-1}(s)W(t)\psi_1(t) |\Psi_1\rangle, \qquad I_2(s, t) = \langle\Psi_2| R^{-1}(s)R(t) |\Psi_2\rangle. \tag{5.13}$$

We have used the fact that the ground state is a product state: $\Psi_0 = \Psi_1 * \Psi_2$ where Ψ_1 is a state of the "1" field and Ψ_2 is a state of the "2" field. Ψ_1 is filled with b particles up to $+k_F$ and has no c particles; Ψ_2 is filled with b particles down to $-k_F$ and has no c particles.

Now, using the definition (5.8) and the rule (5.10) we easily find that

$$W^{-1}(s)W(t) = W_-(s, t)W_+(s, t)Z_1(s, t), \tag{5.14}$$

with

$$W_+(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_1(-p)[\cosh \varphi(p) - 1] \times p^{-1}(e^{ipt} - e^{ips})\},$$

$$W_-(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_1(p)[\cosh \varphi(p) - 1] \times p^{-1}(e^{-ips} - e^{-ipt})\},$$

$$Z_1(s, t) = \exp\{2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1]^2 \times p^{-1}(e^{ip(s-t)} - 1)\}. \tag{5.15}$$

Likewise,

$$R^{-1}(s)R(t) = R_-(s, t)R_+(s, t)Z_2(s, t), \tag{5.16}$$

with

$$R_+(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_2(p)[\sinh \varphi(p)] \times p^{-1}(e^{-ips} - e^{-ipt})\},$$

$$R_-(s, t) = \exp\{2\pi/L \sum_{p>0} \rho_2(-p)[\sinh \varphi(p)] \times p^{-1}(e^{ipt} - e^{ips})\},$$

$$Z_2(s, t) = \exp\{2\pi/L \sum_{p>0} [\sinh \varphi(p)]^2 \times p^{-1}(e^{ip(t-s)} - 1)\}. \tag{5.17}$$

We see at once from the definition (3.1b), (3.2b), of $\rho_1(p)$ that, for $p > 0$, $\rho_1(-p) |\Psi_1\rangle = 0$. Similarly $\langle\Psi_1| \rho(p) = 0$, $\rho_2(p) |\Psi_2\rangle = 0$, and $\langle\Psi_2| \rho_2(-p) = 0$. Hence,

$$I_2(s, t) = Z_2(s, t)$$

and

$$I_1(s, t) = Z_1(s, t)\langle\Psi_1| W_-^{-1}\psi_1^+(s)W_-W_+\psi_1(t)W_+^{-1} |\Psi_1\rangle. \tag{5.18}$$

If we now define

$$h_+(y) = 2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1] \times p^{-1}(e^{ipt} - e^{ips})e^{-ipy},$$

$$h_-(y) = 2\pi/L \sum_{p>0} [\cosh \varphi(p) - 1] \times p^{-1}(e^{-ipt} - e^{-ips})e^{ipy}, \tag{5.19}$$

combining (3.10) and (5.15) we have that

$$W_+(s, t) = \exp \int_0^L N_1(y)h_+(y)\, dy, \qquad W_-(s, t) = \exp -\int_0^L N_1(y)h_-(y)\, dy. \tag{5.20}$$

Since

$$[\psi_1(x), N_1(y)] = \delta(x - y)\psi_1(x), \qquad [\psi_1^+(x), N_1(y)] = -\delta(x - y)\psi_1^+(x), \tag{5.21}$$

it follows that

$$W_+(s, t)\psi_1(t)W_+^{-1}(s, t) = \psi_1(t) \exp[-h_+(t)], \qquad W_-^{-1}(s, t)\psi_1^+(s)W_-(s, t) = \psi_1^+(s) \exp[+h_-(s)]. \tag{5.22}$$

Finally,

$$\langle\Psi_1|\ \psi_1^+(s)\psi_1(t)\ |\Psi_1\rangle = 1/L \sum_{p\leq k_F} e^{ip(t-s)} \equiv Z_3(s,t). \tag{5.23}$$

Combining all these results, we conclude that

$$I(s,t) = Z_0(s,t)Z_1(s,t)Z_2(s,t)Z_3(s,t), \tag{5.24}$$

where

$$Z_0(s,t) = \exp(h_-(s) - h_+(t)) = \exp\{-4\pi/L \sum_{p>0} [\cosh\varphi(p) - 1] \times (1 - e^{ip(s-t)})\}. \tag{5.25}$$

In order to make a comparison with Luttinger's calculation of $\bar{n}_k$, we first observe that the functions $Z_i(s,t)$ are really functions of $r = s - t$ and that they are periodic in s and t in $(0, L)$. We then define the functions $G(r)$ and $Q(r)$ as follows:

$$\exp[-Q(r)] \equiv G(r) \equiv Z_0(r)Z_1(r)Z_2(r). \tag{5.26}$$

Substituting (5.26), (5.24), and (5.23) into (5.2) we obtain

$$\bar{n}_k = 2\pi/L \sum_{p\leq k_F} F(k-p), \tag{5.27}$$

where

$$F(k) = 1/2\pi \int_{-\frac{1}{2}L}^{\frac{1}{2}L} dr\, e^{ikr} e^{-Q(r)} \tag{5.28}$$

$$\cong 1/2\pi \int_{-\infty}^{\infty} dr\, e^{ikr} e^{-Q(r)}. \tag{5.29}$$

In (5.29) we have passed to the bulk limit N, $L \to \infty$, not an approximation.

At this point our expression for $\bar{n}_k$ is formally the same as Luttinger's [cf. L (52), L (69)]. The difference is that our Q is different from his. He obtains Q by evaluating an infinite Toeplitz determinant with the result that [L (70)]

$$Q(r) = \lambda^2/2\pi^2 \int_0^\infty dp\, \frac{1-\cos pr}{p} |v(p)|^2. \quad \text{(Luttinger)} \tag{5.30}$$

Our Q, which is the correct one to use, is obtained by combining (5.15), (5.17), and (5.25), replacing sums by integrals in the usual way, and using the definition (4.11) of $\varphi(p)$. The result is

$$Q(r) = \lambda^2/2\pi^2 \int_0^\infty dp\, \frac{1-\cos pr}{p} |u(p)|^2, \tag{5.31}$$

where

$$|u(p)|^2 = (2\pi^2/\lambda^2)\{(1 - (\lambda v(p)/\pi)^2)^{-\frac{1}{2}} - 1\}. \tag{5.32}$$

It is worth noting that (5.30) agrees with (5.31) to leading order in λ^2.

Since we have not yet specified $v(p)$, we may now follow Luttinger's discussion from this point on with the proviso that we use the correct (λ dependent) $u(p)$ instead of $v(p)$. The reader is referred to pages 1159 and 1160 of Luttinger's paper.

There are two main conclusions one can draw. The first is that if we start with a δ-function interaction [so that $v(p)$ and hence $u(p)$] are constants, it can be shown that $\bar{n}_k = \frac{1}{2}$ for all k. Such a result is quite unphysical, but it is not unreasonable because the ground-state energy W (4.13a) diverges when $v(p) =$ constant at large p. Also, the result would be the same if we started with the more physical interaction

$$H' = 1/L \sum_p \{\rho_1(p) + \rho_2(p)\}\{\rho_1(-p) + \rho_2(-p)\}v(p)$$

discussed in the Appendix. This is indeed unfortunate, because relativistic field theories usually begin with local (δ-function) interactions.

The second conclusion is that if one makes a reasonable assumption about $v(p)$, and hence about $u(p)$ and $Q(r)$, one finds that for k in the vicinity of k_F, $\bar{n}_k$ behaves like

$$\bar{n}_k \sim d - e\,|k - k_F|^{2\alpha}\,\sigma(k - k_F), \tag{5.33}$$

where

$$\sigma(k) = 1, \quad k > 0; \qquad = -1, \quad k < 0 \tag{5.34}$$

and d, e, and α are certain positive constants. Now in Luttinger's calculation

$$\alpha = \lambda^2/4\pi^2 v(0)^2, \quad \text{(Luttinger)} \tag{5.35}$$

[cf. L(75)], where $v(0) \equiv \lim_{p\to 0} v(p)$.

If $2\alpha < 1$, then the conclusion to be drawn is that although the interaction removes the discontinuity in $\bar{n}_k$ at the Fermi surface, we are left with a function that has an infinite slope there. There is, so to speak, a residual Fermi surface. In Sec. IV of his paper, Luttinger shows that at least for one example of $v(p)$ perturbation theory gives the same qualitative result as (5.33) with the same value of α, (5.35).

If, on the other hand, $2\alpha > 1$ then there is no infinite derivative at the Fermi surface. $\bar{n}_k$ is perfectly smooth there (although, technically speaking, it is nonanalytic unless $2\alpha =$ odd integer.) In this case virtually all trace of the Fermi surface has been eliminated. But notice that the correct α to use is obtained by replacing $v(0)$ by $u(0) \equiv \lim_{p\to 0} u(p)$ in (5.35), i.e.,

$$2\alpha = \{1 - [\lambda v(0)/\pi]^2\}^{-\frac{1}{2}} - 1. \quad (5.36)$$

Thus, even subject to the requirement that $|\lambda v(0)|$ be less than π, 2α can become as large as one pleases. Yet perturbation theory predicts (5.35) which yields 2α always less than $\frac{1}{2}$.

We may conclude that a strong enough interaction can eliminate the Fermi surface, while perturbation theory predicts that is always there.

VI. DIELECTRIC CONSTANT

Because the response to external fields of wave vector q only depends on an interaction expression linear in the density operators, we can immediately obtain for the generalized static susceptibility function or *dielectric constant* (response ÷ driving force), for any temperature, T

$$\chi_\lambda(q, T) = \chi_0(q, T)\{\sinh \varphi(q) + \cosh \varphi(q)\}^2 \cosh 2\varphi_q$$
$$= \chi_0(q, T) \frac{1}{1 + \lambda v(q)/\pi} \quad (6.1)$$

in terms of the "unperturbed" susceptibility $\chi_0(q, T)$. It is also a simple exercise to calculate exactly the time dependent susceptibility in terms of the "unperturbed" quantity.

It is interesting to note that the susceptibility can diverge (which is symptomatic of a phase transformation) only for

$$\lambda v(q) \to -\pi, \quad (6.2)$$

i.e. only for sufficiently *attractive* interactions and not for repulsive [$v(q) > 0$] interactions.

Recently Ferrell[6] advanced plausible arguments why a one-dimensional metal cannot become superconducting. We can prove this rigorously in the present model. The electron–phonon interaction is

$$H_{el-ph} = \sum_p g(p)[\rho_1(p) + \rho_2(p)]\cdot[\xi_p + \xi^+_{-p}], \quad (6.3)$$

where ξ and ξ^+ are the phonon field operators. In the "filled-sea" limit this coupling is bilinear in harmonic-oscillator operators, and therefore the Hamiltonian continues to be exactly diagonalizable. The new normal modes can be calculated and there is found to be no phase transition at any finite temperature.

APPENDIX

We shall be interested in extending Luttinger's model in two ways. Firstly, we note that the restriction $\bar{V} = 0$ is really not necessary. Turning back to Eqs. (2.13) *et seq.* we impose periodic boundary conditions $\Psi(\cdots, x_i + L, \cdots) = \Psi(\cdots, x_i, \cdots)$, and find that

$$(q + N\lambda\bar{V}) \text{ and } (k + M\lambda\bar{V}) = 2\pi/L \times \text{integer} \quad (A1)$$

replace the usual condition (2.16), where N = number of "1" particles and M = number of "2" particles. However, when $N, M \to \infty$ in the field-theoretic limit the problem evidently becomes ill-defined unless $\bar{V} \equiv 0$.

A less trivial observation concerns the form of the interaction potential. There is no reason to restrict it to the form $\propto \rho_1\rho_2$, and in fact the more realistic two-body interaction

$$H' = \frac{\lambda}{L} \sum_p v(p)\{\rho_1(-p) + \rho_2(-p)\}\{\rho_1(p) + \rho_2(p)\} \quad (A2)$$

is fully as soluble as the one assumed in the text, for any strength positive $v(p)$, and provided only

$$\lambda v(p) > -\tfrac{1}{2}\pi, \quad (A3)$$

i.e. provided no Fourier component is *too* attractive. The shift in the ground-state energy is now given by

$$W_2 = \sum_{p>0} p\left\{\left(1 + \frac{2\lambda v(p)}{\pi}\right)^{\frac{1}{2}} - 1\right\}. \quad (A4)$$

The plasmon energy is now

$$\epsilon''(p) \equiv |p|\,(1 + 2\lambda v(p)/\pi)^{\frac{1}{2}} \quad (A5)$$

and *for the important case of the Coulomb repulsion*, $v(p) = p^{-2}$, the plasmons describe a relativistic boson field with mass

$$m^* \equiv (2\lambda/\pi)^{\frac{1}{2}} \quad (A6)$$

and dispersion

$$\epsilon''(p) = (p^2 + m^{*2})^{\frac{1}{2}}. \quad (A7)$$

Here, too, $d\epsilon''/dp < 1$.

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Selecta of Elliott H. Lieb
Edited by B. Nachtergaele, J. P. Solovej and J. Yngvason

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Statistical Mechanics
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